A Study on how an Environment Influences Quantum Thermalization in the Dicke Model

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“Stay awhile and listen” - Deckard Cain (Diablo)

Abstract

This thesis will examine the interaction between an isolated chaotic quantum system and an environment. An example of a chaotic quantum system is the Dicke model, describing the interaction of a collection of two-level atoms with a radiation field. For environment, two different case are considered, corresponding to dissipation into an external radiation field, or a measuring surrounding which acts to determine one of the conjugate operators representing position or momentum. It is in this setting the phenomena of quantum thermalization is investigated. In order to study this, a quasi-distribution is used in phase space. From this examination, the non-intuitive conclusion is reached that a system in contact with an environment does not necessarily have to reach steady state (thermalize) faster than it would if it were isolated.

Sammanfattning

I den här avhandlingen undersöks växelverkan mellan ett isolerat kaotiskt kvantmekaniskt system och en omgivning. Ett exempel på ett kaotiskt kvantmekaniskt system är Dicke-modellen, som beskriver växelverkan mellan en samling av två-nivå-atomer och ett elektromagnetiskt fält. Som omgivning tas två olika fall, svarande mot dissipation från systemet in i ett yttre elektromagnetiskt fält, eller en mätningsomgivning som verkar för att bestämma en av de konjugerade operatorerna som representerar position eller rörelsemängd. Det är mot denna bakgrund som undersökningen av fenomenet kvant-termalisering genomförs. För att kunna studera detta så nyttjas en kvasi-fördelning i fasrummet. Från denna granskning nås den icke-intuitiva slutsatsen att ett system i kontakt med en omgivning inte nödvändigtvis måste nå fortvarighetstillstånd (termaliseras) snabbare än om systemet hade varit isolerat.

Acknowledgements

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Contents

Part I
Introduction

“Louis, I think this is the beginning of a beautiful friendship” - Rick Blaine (Casablanca)

1 Introduction

In this thesis we will concern ourself with the examination of the interplay between quantum chaos and open systems. It is in this intersection we will discuss contradictory results stemming from a combination of effects related to open systems and closed chaotic systems. From the consideration of an open system we know that this connection causes decoherence [1], one of the cornerstone in the explanation how the classical macroscopic world emergences from the microscopical one. The connection of an isolated system with an environment promotes the transition from quantum to classical. But this is not the only effect which can be identified as resulting from this consideration.

Even tough quantum physics often is considered unintuitive compared to classical mechanics we still expect some of its characteristics to hold true. For example, a system should reach equilibrium faster when in contact with a thermal bath than it would if it where to be isolated. This is predicted by the laws of thermodynamics [2]. Hence, we assume that an open system reach thermal equilibrium faster than a closed one. We will, however, see that this is not strictly the case.

Where open systems can be considered fairly well understood, quantum chaos is a bit more problematic. The chief reason for that is that the most defining trait of classical chaos, the sensitivity to perpetuated initial conditions, fails to manifest itself in any clear way in quantum mechanics. Still, advances in understanding quantum chaos took place in the 70s and 80s and today general results do exist [3]. Yet, no clear definition is in use for what one means when talking about quantum chaos and some researcher avoid the name entirely[1]. Emulating classical statistical mechanics we expect that chaos is needed for a system to reach thermal equilibrium. This may seem strange as chaos are not that often discussed, but the fact is that chaos is the rule rather then the exception for generic dynamical systems. Therefore, the study of quantum chaotic systems is of interest to determine whether a system thermalizes or not [4]. Quantum systems which are not chaotic (or more preciously are integrable) do not thermalize according to the model used here. Luckily, most physical systems outside the laboratory are complex to such a degree that chaos can be expected. It is important to stress already now that quantum integrability is not a well defined concept and systems that by all account should be non-integrable (according to definitions in practice) and thermalize, fail to do so[2]. Yet, even though the certainty that quantum

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[1] Often weasel words are used like: quantum “signatures” of chaos, quantum “manifestions” of chaos, or quantum chaology. We will unavoidably adhere to use these terms at times.

[2] The implication is that systems which exhibit quantum chaos sometimes fail to thermalize in a quantum sense. This is in sharp contrast to the classical sense where every system which is chaotic

chaos implies thermilzation is in question, the two concepts should in all likelihood be related in some manner. What is a bit staggering is that without a clear understanding of quantum thermalization we cannot speak about, for example, such a familiar concept as temperature!

Aside from answering fundamental questions considering quantum theory, this is also of interest to future applications, such as quantum computers. Any practical quantum computer must consist of a large number of qubit. The Hamiltonian describing them could in all likelihood be complex in the sense that it is non-integrable and furthermore, chaotic. It is of interest to examine if these quantum chaotic effects hampers efforts to construct quantum computers in practice.

To study this we will pick a system which is known to exhibit quantum chaos when isolated. This system is described by the *Dicke Hamiltonian* [5]. We will then couple this system to an environment. Two kinds of environment will be considered, constituting a radiation field and a "measuring" bath. From this we will examine various properties for the system and how it is affected by the coupling to the environment. Most prominent will be investigation of what is known as the quasi probability distribution, charactering the state of the system.

In order to carry out this analysis we will work with a certain formulation of quantum mechanics, valid in phase space. This framework is known as the *phase space formulation of quantum mechanics*. The reason for picking this representation over the well known operator formalism is because of its advantage in visualising states directly in phase space. The fact that we can represent states and operators in phase space makes the connection to classical chaos all that more apparent, meaning that the phase space formulation of quantum mechanics is the best choice for studying quantum chaos and decoherence.

1.1 Outline

The structure of the thesis is constructed in such a way that it consists of three parts. The first part is the present, the introduction. The second is the theory part, which is the largest. Part two is in turn split up into three distinct chapters, each treating one of the major subjects touched upon in this thesis. Chapter two discusses the phase space formulation of quantum mechanics, and is by itself the longest chapter in the thesis. Following that is chapter three which is a quick overview of the theory concerning open quantum systems. Lastly is chapter four which deal with the concept of chaos, both in the classical world as-well as in quantum mechanics. In part three we present derivations, results and analysis concerning the problem set-up. As can be already

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must thermalize.

guessed from the introduction, the style throughout this thesis will be informal. The reason for this is to make the text more pedagogical, as an informal text almost always is easier to follow and learn from.

Before ending this section a few words about the scope of the thesis are appropriate. The author strived to make the thesis self-contained to the largest extent as possible. A consequence of this is that the thesis is possibly longer than a typical one. Still, it is the authors opinion that the concept of "self-contained" is a goal which should always be desired. Hence, this thesis can hopefully be read and understood by readers with a diverse background, only requiring basic knowledge in ordinary quantum mechanics. For the reader already familiar with any of the subjects touched upon in the theory section, those chapters can be skipped. For example, if the reader already know about open quantum systems that chapter can be omitted. With that said, it is the authors belief that especially chapter two contains material preciously unknown for the majority of the readers[3].

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[3] Even if the reader knowns about the phase space formulation of quantum mechanics the presentation of this subject in chapter two is one which is not commonly encountered.

Part II

Theory

"It can scarcely be denied that the supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience" - Albert Einstein

2 The Phase Space Formulation of Quantum Mechanics

In this chapter the theory of the phase space formulation of quantum mechanics (PSQM) will be presented. The treatment will not make any claim to be mathematically rigorous. For this to be the case a different approach based on differential geometry and group theory is needed [6]. Still, the methods employed in this thesis are sufficient for most uses. The structure will in some ways be unique in the sense that it will combine many different approaches to the subject into a hopefully coherent combination, but we are greatly inspired by the presentation in [7]. To often is the presentation of this specific subject ill explained and mistreated. The Wigner function is often presented without any arguments what so ever and the reader is forced to accept that it is based on sound grounds only by assumption. There is however a better way. Staring from a more rigorous mathematical framework (which it actually is) we can, by beginning from very general quantum mechanical relations, derive the entire formalism in a way where it is transparent that it conveys all the results of quantum theory. With that said, it is important to stress the fact that we will try to avoid getting caught up in technical details when dealing with the underlying mathematical framework. The PSQM is a result of a more general mathematical theory dealing with quantization called *deformation quantization*, but here we leave the unnecessary (for us here) details to the mathematicians.

PSQM is used in several distinct fields of physics, with the most common being quantum optics.

The outline of this chapter is as follows: First we will motivate and explain the need and strength of the PSQM and how it will be imperative to the study of decoherence and chaos. After that we start the outline of the theory by examining the simple problem of relating an operator to a function, and then quickly realise how the next problem of two operators cause direct headache as a consequence of ordering ambiguity. In the sections following we examine the Weyl correspondence as well as the Weyl ordering of operators and how this ultimately results in the Wigner function. Before exploring properties of the Wigner function, the important question of non-commutative in PSQM is explored and the result is what is known as the star product between phase space functions. After a short interlude on the subject of coherent states we present another phase space distribution called the Husimi function (or simply Q-function). We also illustrate the change from position and momentum operators in the Winger function to creation and annihilation operators. We close this chapter by considering the laborious topic of spin in the PSQM.

2.1 Why Another Formulation?

When, as a young student, one begins to learn quantum mechanics the approach is largely the same for everybody. First one is introduced to the Schrödinger picture by virtue of simply postulating the Schrödinger equation and the wave function which fully describes the physical system. After a brief period of time one is introduced to the Heisenberg picture and its corresponding evolution equation along with the more abstract notion of state vectors and the "bra-ket" notation. In more advanced courses and settings, one inevitably encounter the Path integral ("sum over histories") formulation. For most this is the end point of exposure to the underlying formulation of quantum theory, the rest is application to different systems and scenarios. Often overlooked is the phase space formulation of quantum mechanics, which is relegated to the side-line where it has to wait indefinitely to be tagged in. But no more will this be the case! In this thesis the star will be the phase space formulation (this pun will become clear latter).

To motivate further study of the PSQM we first have to answer the burning question of why we should bother with another formulation when we already have several others eagerly waiting to be used and applied. To illustrate this recall the various formulations of classical mechanics. For beginners Newtonian mechanics is the easiest and can with easy be visualized to get a grasp of the problem. Newtonian mechanics is however ill suited for handling more advanced situations where for example constraints are necessary to describe the motion of a particle. In these scenarios Lagrangian mechanics is far superior. Moreover, Newtonian mechanics is notoriously bad at treating and describing chaos[4], where instead Hamiltonian mechanics[5] excel. In spite of this the most important reason for choosing one formulation over another is often which one results in the easiest calculations, in the same way you want to avoid unnecessary cumbersome calculations by working in a suitable coordinate frame. Another option is to work in the formulation which yields the simplest or clearest interpretation of a physical phenomena along with a deeper understanding. Many of these arguments finds analogy in quantum mechanics and the different formulations. There is however one major difference and that is the question of how to relate the quantum theory to classical mechanics (the classical limit).

To recap, we have three working formulation of quantum mechanics [6]. In table 1 we list all the formulations along with some of their strengths and weaknesses. The

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[4] The natural setting to discuses chaos is by visualising process in phase space.

[5] Hamiltonian mechanics can also treat open systems where the conservation of phase space volume no longer needs to be true.

[6] The Schrödinger and the Heisenberg-picture are sometimes grouped together into one formalism [8]. The reason for this is the common mathematical structure underlying the two formulations [9].

Formulations of Quantum Mechanics		
Formulations	Strengths	Weakness
1. **Schrödinger/Heisenberg** Mathematical Space: • Configuration (Wave Functions) • Hilbert (Operators)	• Comparatively easy mathematically • Often the easiest to interpret	• Not always a well defined classical limit • Problem dealing with constraints
2. **Path Integral** Mathematical Space: • Euclidean	• Good at dealing with (gauge) constraints	• Comparatively cumbersome mathematically
3. **Phase Space** Mathematical Space: • Phase (Quasi-distributions)	• Ability to visualise states • Well defined classical limit	• Comparatively cumbersome mathematically • Comparatively underdeveloped

Table 1: The different formulations of quantum mechanics. In this table the Schrödinger and Heisenberg-pictures are presented as a common formulation. The reason for this is to emphasise the close connection between the two.

PSQM possess primarily two advantages over the other formulations besides the fact that it is valid in both the position and momentum domain (space) at the same time without the need to perform cumbersome transformations. In particular, it has the ability to visualize the states directly in phase space. This is especially useful when dealing with interference or superposition, or when relating it to the other strength of the PSQM, namely its relation to the classical limit. The other advantage of PSQM is the more direct connection to classical statistical mechanics. We will se later that both the Wigner function (the PSQM analogy to the wave function) and its corresponding evolution equation have natural classical limits in the form of classical statistical phase space distributions and Liouville's equation in the case of the evolution equation. The ability to visualise the states along with the more readably applied classical limits makes the PSQM the natural choice for studying chaos and decoherence.

2.2 The Heart of Quantum Mechanics: The Canonical Commutation Relation

When crossing from the familiar realm of classical mechanics into the "strange" world of quantum mechanics one have to renounce many central ideas hold dear in the classical theory. Among them, two are the most obvious departures from our intuitive picture of how the physical world works. First we have to accept the fact that our theory no longer has the power to predict each and every outcome with certainty, only the probability that a certain event transpire. This is captured in the probabilistic nature of the wave function. Secondly we have to come to terms with the ramification that we cannot measure all our usual observables at the same time with unchanged precision. This ramification is a consequence of the *canonical commutation relation* between conjugate variables and will now be examine in somewhat detail.

The position/momentum canonical commutation relation[7] is usually stated as

$$\hat{x}\hat{p} - \hat{p}\hat{x} = [\hat{x}, \hat{p}] = i\hbar. \tag{2.1}$$

This form is flawed from a mathematical stance since we have a product of operator on one side and a number on the other. More correctly this relation should be stated as

$$[\hat{x}, \hat{p}] = i\hbar\mathbb{1}, \tag{2.2}$$

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[7] Some authors reserve the name "canonical" commutation relations to those where the commutator (measure of non-commuting) is a number. This is in contrast to for example angular momentum where the commutator is equal to a operator.

where $\mathbb{1}$ is the identity operator. The canonical commutation relation is a statement on how $\hat{x}$ and $\hat{p}$ fails to be interchangeable in order when intended to operate on a state/wave-function. That is to say that first measuring the position and then the momentum is not the same as first measuring the momentum and then the position. This is akin to rotation in 3-dimensions, where rotation around one axis followed by another rotation around a different axis is not identical to the procedure performed the other way. In fact, the canonical commutation relation is the reason for the inability to exactly measure both the position and momentum of a particle at the same time [10]. This uncertainty relation is of course nothing else then the famous *Heisenberg's uncertainty relation* but it is interesting to note that this relation is only a consequence of the more general result which is the canonical commutation relation.

It is known that the realisation of $\hat{x}$ and $\hat{p}$ is symmetric in the sense that if we work in position representation we have that the operators can be expressed as

$$\hat{x}_{position} \rightarrow x \qquad \text{and} \qquad \hat{p}_{position} \rightarrow -i\hbar\frac{\partial}{\partial x}, \tag{2.3}$$

while in momentum representation

$$\hat{x}_{momentum} \rightarrow i\hbar\frac{\partial}{\partial p} \qquad \text{and} \qquad \hat{p}_{momentum} \rightarrow p. \tag{2.4}$$

Regardless of which we choose Eq.(2.2) remains true; the action of $\hat{x}$ on a position wave function is mirrored by the action of $\hat{p}$ on a *momentum wave function* which is provided by the connection of Fourier transformation.

Eq.(2.2) is not only true for position and momentum but for any pair of operators corresponding to observables whose classical counterparts are conjugate variables[8]. Thus we can already tentative make a guess that the Fourier transformation (which is the connection between a pair of conjugate variables) may play a role in our attempt to formulate quantum mechanics in phase space, that is to say if we still want to acknowledge the uncertainty principle; which all experiment points at that we should. Indeed, we will in the next section see that the key component to associating operators and ordinary functions is done by utilizing the Fourier transformation.

Even though Eq.(2.2) appears at first glance to be a sound statement mathematically it can be shown relatively easy that it is plagued by some shortcomings. To start with we recall that Eq.(2.2) is a operator relation[9] and should thus be understood as

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[8] Conjugate variables are variables (of two) that are connected to each other by Fourier transformation.

[9] This equation could also be realised as a matrix relation. Then the operators are represented in a choose base as matrices and the product is simply a matrix product. Still, to always reference a base is something that we want to avoid to make the statement as general as possible.

operating on a state/wave function. Already at this point we can distinguish one not to pleasant detail. The right hand side of Eq.(2.2) just contains the identity operator and is well defined for every member of the Hilbert space (for every conceivable state). However, the left hand side contains derivatives, regardless in which representation one works in. By considering a state which is not analytical it is possible to break this equality. If such a state can be physical or not is for the purposes of this thesis not important. In addition we can show that if $\hat{x}$ and $\hat{p}$ together are to satisfy Eq.(2.2) then they cannot both be bounded operators [6, 9]. This is a problem from a mathematical viewpoint as many theorems in functional theory rest on the assumption of bounded operators [11].

For us pragmatical physicists this is not something to be terribly alarmed about. Ordinary quantum mechanics represented by either Schrödingers wave mechanics or Heisenberg's matrix mechanics produce results which agrees well with experiments. It can, nonetheless, be instructive to consider a rewriting of the canonical commutation relation in a form which remedy these concerns. Moreover, any reformulation of a known physical relation can ideally result in a form which leads itself to new physical insight. To consider any modification to Eq.(2.2) we have to ensure that the modified form produces the same predictions for experiments and under suitable relaxed conditions reduces to the original commutation relation.

The procedure to modify Eq.(2.2) is credited to Weyl [12] and consists of rewriting it in an exponential form with only unitary operators. To do this we define

$$U(s) = e^{is\hat{p}}$$

and

$$V(k) = e^{ik\hat{x}}$$

which are constrained to satisfy

$$U(s)V(k) = e^{isk}V(k)U(s). \tag{2.5}$$

$U(s)$ and $V(k)$ are one-parameter groups that must obey the relation Eq.(2.5), thus it is important to note that Eq.(2.5) is not a general result that holds for all one parameters unitary groups but only for those that are constructed from operators satisfying Eq.(2.2) [9]. If it is assumed that $\hat{x}$ and $\hat{p}$ are bounded operators then we can Taylor expand $U(s)$ and $V(k)$ to re-obtain the original formulation.

Related to Eq.(2.5) (known as the Weyl form of the canonical commutation relations[6]) are the following operators[10] which "constitute a projective unitary representation" of

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[10] In a general context operators on this form which also satisfy some properties [6][9] are sometimes called Weyl operators. We will reserve that name for other objects which we will encounter later.

said relation

$$\omega(\hat{x}, \hat{y}) = e^{i\theta\hat{x}+i\tau\hat{p}}, \tag{2.6}$$

where it is assumed that the parameters either are fixed or are to be integrated over. These operators are of fundamental importance when formulating quantum theory in a mathematically rigours way [9]. It is important to note that $e^{i\theta\hat{x}+i\tau\hat{p}}$ does not imply that $e^{i\theta\hat{x}}e^{i\theta\hat{p}}$, that is only true for operators that commute. In a manner of speaking we can say that the $\omega(\hat{x}, \hat{y})$ summarise the canonical commutation relation if we keep the non-commuting detail of referred operators in mind (this should not be taken to literal). $\omega(\hat{x}, \hat{y})$ is important as it will be a stepping stone when formulating the Weyl correspondence as it will natural emerge when we strive to formulate quantum mechanics in phase space. The expectation value of this operator is known as the (quantum) *characteristic function* and can be used to obtain the quantum quasi-distribution in the same way as in the classical theory. Before discussing how to associate a function characterised by two variable to a given operator we first treat the much more simple case of a single operator and a function of a single variable.

2.3 Association Between Operators and Ordinary Functions

Before discussing the association (or correspondence) between operators and functions we first state a couple of important properties that will become useful. To start with we have to realise that a function of operators is not necessarily well defined; what does it mean for $e^{\hat{x}}$ to act on a function $f(x)$? This issue is often resolved by *defining* a function of an operator $f(\hat{x})$ as the power series expansion of the original function $f(x)$

$$f(x) = \sum_{n=0}^{\infty} f_n x^n \tag{2.7}$$

and then replacing the ordinary variable x with the desired operator

$$f(\hat{x}) = \sum_{n=0}^{\infty} f_n \hat{x}^n. \tag{2.8}$$

The process of replacing a variable with a operator can also be performed in other areas. For example, another approach is by considering the Fourier transform of our original function $f(x)$

$$\tilde{f}(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)e^{-ixp}dx \tag{2.9}$$

and then from this define

$$f(\hat{x}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(p) e^{ip\hat{x}} dp \tag{2.10}$$

which is the inverse Fourier transform of the original function where we have replaced x with the operator $\hat{x}$. Eq.(2.10) is not a immediate solution on how to treat operator functions but is of indispensable value as the operator function dependency for an arbitrary operator valued function is shifted to the exponential factor. These are the two most important relations for us concerning operator functions[11].

We will also make extensive use of the special form of the Baker–Campbell –Hausdorff formula for exponentials containing operators

$$e^{\hat{A}+\hat{B}} = e^{-\frac{1}{2}[\hat{A},\hat{B}]} e^{\hat{A}} e^{\hat{B}} = e^{\frac{1}{2}[\hat{A},\hat{B}]} e^{\hat{B}} e^{\hat{A}}, \tag{2.11}$$

which is valid if $[[\hat{A}, \hat{B}], \hat{A}] = [[\hat{A}, \hat{B}], \hat{B}] = 0$. For $[\hat{x}, \hat{p}] = i\hbar$ the commutator is only a number and this form is valid.

In this chapter we will work in units where $\hbar = 1$. In a later section we will examine where the occurrence of $\hbar$ will affect our results when we take $\hbar \to 0$ which in PSQM is the well defined classical limit.

2.3.1 Elementary Example: One Operator, One Variable

To get used to the idea of associating operators with functions we start by consider the simple case of only a single operator. Suppose that we want to calculate the expectation value of the position for a particle

$$\langle \hat{x} \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{x} \psi(x) dx = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx, \tag{2.12}$$

where the last step is possible because x is the eigenvalue to $\hat{x}$ in position space. This exception value must yield the same result in momentum space for the result to be independent of our choice of representation.

$$\int_{-\infty}^{\infty} x |\psi(x)|^2 dx = \int_{-\infty}^{\infty} \tilde{\psi}^*(p) \hat{x} \tilde{\psi}(p) dp \tag{2.13}$$

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[11] This is a truth with modifications, the delta function definition is also encountered and used in some sources. This one usually emerge when one first use the Fourier transform definition and then use the integral form of the delta function. The result is often something on the form of $\delta(x - \hat{x})$. In that way one can think of it as a derived result even though one can also define this operator form from the start.

with $\tilde{\psi(p)}$ the Fourier transform of $\psi(x)$

$$\tilde{\psi(p)} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x) e^{-ixp} dx. \tag{2.14}$$

In the right hand side of Eq.(2.13) we cannot make the same simplification as in Eq.(2.12) because now $\hat{x}$ does not act on eigenstates. Instead we are left with $\hat{x}$ sandwiched in the middle of the two state functions. If we generalise this result to an arbitrary function of the operator $f(\hat{x})$ we obtain

$$\int_{-\infty}^{\infty} f(x) |\psi(x)|^2 dx = \int_{-\infty}^{\infty} \tilde{\psi}^*(p) f(\hat{x}) \tilde{\psi}(p) dp. \tag{2.15}$$

From this result we can make the trivial association that $f(x)$ in the position domain is related to $f(\hat{x})$ in the momentum (Fourier) domain. We indicate this symbolically as

$$f(x) \leftrightarrow f(\hat{x}). \tag{2.16}$$

In the same way can we establish the association for an arbitrary function of $\hat{p}$ between the position domain and the momentum domain. Moving past the consideration of only one operator we quickly hit a snag.

2.3.2 Several Operators: The Problem of Ordering

Dealing with one operator is simple enough, we just replace the classical variable with its corresponding hermitian operator (or vice versa when going from operator to variable). When considering two non-commuting operators we however encounter the problem of ordering of operators. For example, take the simple case of a classical function depending on the variables x and p, representing position and momentum respectively. The simplest case we can imagine is of the form

$$f(x, p) = xp. \tag{2.17}$$

We can, however, just as well write this as

$$f(x, p) = xp = px = \frac{1}{2}(xp + px). \tag{2.18}$$

These are the three most straightforward ways we can write this form. From a classical viewpoint both these forms are equivalent. If we were to promote $x \to \hat{X}$ and $p \to \hat{P}$ this would no longer be the case, as now $\hat{X}$ and $\hat{P}$ no longer commute. Thus, we are forced to deal with the order ambiguity going from classical variables to operators. The most direct question one can ask is if one of the orderings is preferred over another? The answer turns out to be that every ordering is equally valid within its own framework and that choosing an ordering constitutes one of the pillars of the PSQM. In this thesis we will only examine two, *Weyl ordering* and *anti-normal ordering.* Each ordering is intimately connected to to the quasiprobability distribution that will describe our physical state(s).

2.3.3 The Weyl Correspondence

We now present the procedure to associate an operator valued function $A(\hat{X}, \hat{P})$ with a variable valued "classical" function $a(x, p)$, from now on denoted *c-function* (also called *symbol* by some). From here on out will drop the “hat” notation from operators, capital X and P are to be understood as operators while x and p as ordinary variables. In addition integrals without limits $\int = \int_{-\infty}^{\infty}$ to keep the notation clean.

To start we first define the Fourier transform of $a(x, p)$

$$\tilde{a}(\theta, \tau) = \frac{1}{4\pi^2} \iint a(x, p) e^{-i\theta x - i\tau p} dx dp \tag{2.19}$$

and its inverse

$$a(x, p) = \iint \tilde{a}(\theta, \tau) e^{i\theta x + i\tau p} d\theta d\tau. \tag{2.20}$$

From this we define the associated operator to $a(x, p)$, called the *Weyl operator* $A(X, P)$ by replacing x and p by the operators X and P

$$A(X, P) = \iint \tilde{a}(\theta, \tau) e^{i\theta X + i\tau P} d\theta d\tau. \tag{2.21}$$

Note that the exponential is the same as in Eq.(2.6). By utilising

$$e^{i\theta X + i\tau P} = e^{i\theta\tau/2} e^{i\theta X} e^{i\tau P} = e^{-i\theta\tau/2} e^{i\theta P} e^{i\tau X} \tag{2.22}$$

this can be written as

$$A(X, P) = \iint \tilde{a}(\theta, \tau) e^{i\theta\tau/2} e^{i\theta X} e^{i\tau P} d\theta d\tau \tag{2.23}$$

or

$$A(X, P) = \iint \tilde{a}(\theta, \tau) e^{-i\theta\tau/2} e^{i\theta P} e^{i\tau X} d\theta d\tau. \tag{2.24}$$

If we also substitute in the expression for $\tilde{a}(\theta, \tau)$ we arrive at

$$A(X,P) = \frac{1}{4\pi^2} \iiiint a(x,p) e^{i\theta(X-x)+i\tau(P-p)} d\theta d\tau dx dp \tag{2.25}$$

or alternatively

$$A(X,P) = \frac{1}{4\pi^2} \iiiint a(x,p) e^{i\theta\tau/2} e^{i\theta(X-x)} e^{i\tau(P-p)} d\theta d\tau dx dp. \tag{2.26}$$

The advantage of the Weyl operator is that it is equally valid in position as in momentum space. In fact it is even more general then that and can as a consequence operate on functions given in any representation. This was one of the goals when rewriting the canonical commutation relation; it does not refer to any specific representation of the operators in any particular domain (space).

To obtain the inverse correspondence from operator to c-function we first define a useful method that converts operators to functions for easy manipulations before converting it back to operators. This *rearrangement function* $R(x,p)$ is a vital stepping stone in the procedure to transform from an operator to a c-function. Given a Weyl operator $A(X,P)$ we define $R(x,p)$ as: *the rearrangement of $A(X,P)$ in the way that all P operators are placed to the right of the X operators and then we replace X and P by x and p.* For an explicit form of $R(x,p)$ we consider Eq.(2.23) which satisfy the definition

$$R(x,p) = \iint \tilde{a}(\theta,\tau) e^{i\theta\tau/2} e^{i\theta x} e^{i\tau p} d\theta d\tau, \tag{2.27}$$

the power in the first exponential term can be obtained by acting on the second and third terms by a suitable derivative in the power

$$R(x,p) = \iint \tilde{a}(\theta,\tau) e^{\frac{1}{2i}\frac{\partial^2}{\partial x \partial p}} e^{i\theta x} e^{i\tau p} d\theta d\tau. \tag{2.28}$$

Integration and derivation commutes

$$R(x,p) = e^{\frac{1}{2i}\frac{\partial^2}{\partial x \partial p}} \iint \tilde{a}(\theta,\tau) e^{i\theta x} e^{i\tau p} d\theta d\tau. \tag{2.29}$$

Since the integration is nothing else then the Fourier transformation of $a(x,p)$ we have

$$R(x,p) = e^{\frac{1}{2i}\frac{\partial^2}{\partial x \partial p}} a(x,p). \tag{2.30}$$

If desired we can now re-obtain $A(X,P)$ after evaluation of the derivatives by first moving all the p variables to the right of x variables and then substituting for X and

P. This method can be used to calculate the Weyl operator for a given c-function. The most straightforward way of evaluating Eq.(2.30) is to expand the exponential and letting the resulting derivatives act on $a(x,p)$ until the higher powers yield zero contributions. From this we see the connection between the Weyl operator and the c-function. In particular, both can be used to obtain the rearrangement operator. By using this we will now describe how to get the c-function from a given Weyl operator. The easiest way is simply to solve for $a(x,p)$ in Eq.(2.30) resulting in

$$a(x,p) = e^{-\frac{1}{2i}\frac{\partial^2}{\partial x \partial p}} R(x,p), \tag{2.31}$$

another way is to start from Eq.(2.27) and taking the inverse Fourier transform. From this we can in principle express any quantum mechanical operator[12] as a c-function in phase space.

Eq.(2.31) allows us to represent any and all operators in phase space (again provided they are a function of X and P). The ordering prescription mentioned before is "hard-coded" in this equation. But what ordering does it imply if we are to put it in concrete words? If we consider a simple example where we have the following operator polynomial

$$A(X,P) = P^2X + 2PXP + XP^2. \tag{2.32}$$

Applying Eq.(2.31) to this after rearranging it to satisfy the definition $R(x,p)$ we find that $a(x,p) = 4p^2x$. From this it appears that the Weyl ordering is the ordering where every possible case is taken into consideration. The general proof of this can be formulated by using mathematical induction but we will omit that here. Still, we can formulate the Weyl ordering as *every operator ordering that in the classical limit corresponds to the same form.* That is, when going from variables to operators we add every conceivable way of writing our function and the replace the variables by operators. This is also the reason why Weyl ordering is sometimes referred to as *symmetric ordering* (even though that name can be a bit misleading).

2.3.4 The Wigner Function

Consider again the calculation of an expectation value as in section 2.3.1 but this time for a general operator $A(X,P)$

$$\langle A(X,P)\rangle = \int_{-\infty}^{\infty} \psi^*(x)A(X,P)\psi(x)dx \tag{2.33}$$

---

[12] Any operator which is a function of X or P. Spin and more exotic phenomena are not that easily subdued.

where $\psi(x)$ is the wave function which describes our physical system. We want to investigate the action of the Weyl operator $A(X,P)$ on the wave function $\psi(x)$. Using Eq.(2.23) we have

$$A(X,P)\psi(x) = \iint \tilde{a}(\theta,\tau)e^{i\theta\tau/2}e^{i\theta X}e^{i\tau P}\psi(x)d\theta d\tau, \tag{2.34}$$

in position space $e^{i\tau P}$ is the well known translation operator[13], meaning that we can write this as

$$A(X,P)\psi(x) = \iint \tilde{a}(\theta,\tau)e^{i\theta\tau/2}e^{i\theta X}\psi(x+\tau)d\theta d\tau. \tag{2.35}$$

Using the explicit form of $\tilde{a}(\theta,\tau)$ and employing the properties of the delta function

$$\delta(x-\upsilon) = \frac{1}{2\pi}\int e^{\pm iy(x-\upsilon)}dy \tag{2.36}$$

and

$$f(\upsilon) = \int f(x)\delta(x-\upsilon)dx \tag{2.37}$$

along with a change of variables we arrive at

$$A(X,P)\psi(x) = \frac{1}{2\pi}\iint a((x+\tau)/2,p)e^{i(x-\tau)p}\psi(\tau)d\tau dp. \tag{2.38}$$

This is the action of the Weyl operator when acting on a wave function in position space. It is possible to derive a similar expression for the action on a wave function in momentum space in the same way. With Eq.(2.38) the expectation value Eq.(2.34) becomes

$$\langle A(X,P)\rangle = \frac{1}{2\pi}\iiint \psi^*(x)a((x+\tau)/2,p)e^{i(x-\tau)p}\psi(\tau)dxd\tau dp. \tag{2.39}$$

Transforming the variables x and τ accordingly

$$\tau \to x + \frac{1}{2}\tau \qquad \text{and} \qquad x \to x - \frac{1}{2}\tau \tag{2.40}$$

we can further rewrite the expectation as

$$\langle A(X,P)\rangle = \frac{1}{2\pi}\iiint \psi^*(x-\frac{1}{2})a(x,p)e^{-i\tau p}\psi(x+\frac{1}{2}\tau)dxd\tau dp. \tag{2.41}$$

---

[13] This is easy to show, just Taylor expand $e^{i\tau P} = \sum_{n=0}^{\infty}\frac{(i\tau)^n P^n}{n!}$ and let it act on $\psi(x)$. The result is the same as the Taylor expansion of $\psi(x+\tau)$, a well known result.

The integrand only consist of c-functions and as such we can rearrange them to make the crucial decision of defining the *Wigner function* as

$$W(x,p) = \frac{1}{2\pi}\int \psi^*(x-\frac{1}{2}\tau)e^{-i\tau p}\psi(x+\frac{1}{2}\tau)d\tau. \tag{2.42}$$

With the Wigner function defined our final expression for the expectation value of the operator $A(X,P)$ takes the form

$$\langle A(X,P)\rangle = \int \psi^*(x)A(X,P)\psi(x)dx = \iint a(x,p)W(x,p)dxdp = \langle a(x,p)\rangle\,. \tag{2.43}$$

The right hand side makes no reference at all to operators and mimic the classical expression for calculating the expectation values in statistical mechanics. Here the Wigner function acts as the probability distribution (or "weight" factor) which gives the measure of how much of $a(x,p)$ is in certain regions of phase space. When we examine the properties of the Wigner function later it will, however, turn out that the Wigner function cannot be a true probability distribution in every sense and it is therefore common to denote it as a *quasi-probability distribution.* Even with this shortcoming, the Wigner function is a remarkable tool, containing every bit of information on our physical system as was preciously contained in the wave function or state vector (or later as we will see also for the density operator). Before discussing properties of the Wigner function, we will first address the question on how to treat the product between two Weyl operators. Such an operation will induce a special product on our phase space functions that capture the noncommutative nature of operators directly in phase space.

2.3.5 Products of Phase-Space Functions: The Star Product

To be a fully fledged theory that capture all that is contained in the operator formalism, the PSQM must have an analogy to the commutator between two operators. We expect this because of the vital importance of the commutator in relations such as the Heisenberg equation of motion (or more interestingly, for the von Neumann equation for the evolution of the density matrix) as well as the generalised uncertainty principle. To transfer the commutator we first have to figure out how to create the product of two phase space c-functions when they correspond to non-commuting quantum mechanical operators. This is achieved by considering the product of two Weyl operators, $A(X,P)$ and $B(X,P)$.

$$C(X,P) = A(X,P)B(X,P) = \iiiint \tilde{a}(\theta,\tau)e^{i\theta X+i\tau P}\tilde{b}(\theta',\tau')e^{i\theta' X+i\tau' P} \\ d\theta d\tau d\theta' d\tau' \tag{2.44}$$

where we define $C(X,P)$ as the product of $A(X,P)$ and $B(X,P)$. Now we wish to find the c-function $c(x,p)$ corresponding to this product. Employing the Baker-Campbell-Hausdorff relation

$$e^{i\theta X+i\tau P}e^{i\theta' X+i\tau' P}=e^{i(\theta'\tau-\theta\tau')/2}e^{i(\theta+\theta')X+i(\tau+\tau')P}, \tag{2.45}$$

Eq.(2.44) becomes

$$C(X,P)=\iiiint\tilde{a}(\theta,\tau)\tilde{b}(\theta',\tau')e^{i(\theta'\tau-\theta\tau')/2}e^{i(\theta+\theta')X+i(\tau+\tau')P}d\theta d\tau d\theta' d\tau' \tag{2.46}$$

alternatively

$$C(X,P)=\iiiint\tilde{a}(\theta-\theta',\tau-\tau')\tilde{b}(\theta',\tau')e^{i(\theta'\tau-\theta\tau')/2}e^{i\theta X+i\tau P}d\theta d\tau d\theta' d\tau'. \tag{2.47}$$

From the general form of $C(X,P)$

$$C(X,P)=\iint\tilde{c}(\theta,\tau)e^{i\theta X+i\tau P}d\theta d\tau \tag{2.48}$$

we identify

$$\tilde{c}(\theta,\tau)=\iint\tilde{a}(\theta-\theta',\tau-\tau')\tilde{b}(\theta',\tau')e^{i(\theta'\tau-\theta\tau')/2}d\theta' d\tau' \tag{2.49}$$

and by performing the inverse Fourier transform we obtain the c-function

$$c(x,p)=\iiiint\tilde{a}(\theta,\tau)\tilde{b}(\theta',\tau')e^{i(\theta'\tau-\theta\tau')/2}e^{i(\theta+\theta')x+i(\tau+\tau')p}d\theta d\tau d\theta' d\tau'. \tag{2.50}$$

This can further be expressed in a different way by substituting in the expressions for $\tilde{a}(\theta,\tau)$ and $\tilde{b}(\theta',\tau')$ and performing a number of changes of variables. However, we have a more interesting form in mind which does not rest on rewriting Eq.(2.50)such ways. Instead, exploiting the commutation between the ordinary variables in Eq.(2.50) this can be expressed as

$$c(x,p)=\iiiint e^{i(\theta'\tau-\theta\tau')/2}\tilde{a}(\theta,\tau)e^{i\theta x+i\tau p}\tilde{b}(\theta',\tau')e^{i\theta' x+i\tau' p}d\theta d\tau d\theta' d\tau'. \tag{2.51}$$

But this is almost the product of $a(x,p)$ and $b(x,p)$ with the exception of the term $e^{i(\theta'\tau-\theta\tau')/2}$. This term can be acquired by acting on $a(x,p)$ and $b(x,p)$ in the right order with a exponential containing derivatives in its power:

$$c_{a,b}(x,p) = a(x,p)e^{\frac{i}{2}(\overleftarrow{\frac{\partial}{\partial x}}\overrightarrow{\frac{\partial}{\partial p}} - \overleftarrow{\frac{\partial}{\partial p}}\overrightarrow{\frac{\partial}{\partial x}})}b(x,p) = a(x,p) \star b(x,p), \tag{2.52}$$

where the arrows over the derivative indicate which c-function it is to act on. In Eq.(2.52) we have defined the *star product* $\star$ between $a(x,p)$ and $b(x,p)$. This product is the phase space replacement of the non-commutative product between operators in the Hilbert space formulation. It is directly apparent from Eq.(2.52) that the order of $a(x,p)$ and $b(x,p)$ is important. From the derivation leading to Eq.(2.52) we see that if we exchange the ordering of $a(x,p)$ and $b(x,p)$ we have to change the sign in the exponential, this is an important property to keep in mind when performing calculations.

In this language we express the commutator as

$$a(x,p) \star b(x,p) - b(x,p) \star a(x,p) = \{a(x,p), b(x,p)\}_{MB} \tag{2.53}$$

where $\{...,...\}_{MB}$ is known as the *Moyal bracket*(MB) [7, 13] between two phase space c-functions. This is the Wigner transform of the ordinary commutator bracket. By using this we obtain the equation of motion for the Wigner function from the von Neumann equation for the density matrix.

We now possess the three pillars of the PSQM, the correspondence rule for going between variables and operators (Weyl ordering), the quasi-distribution function (the Wigner function) and the product rule for c-functions (the star product). In fact the star product contains the ordering prescription discussed earlier. If we have two operators in the form XP we can just replace them by their variable counterpart *but* leaving the implied product between them intact in phase space

$$XP \leftrightarrow x \star p. \tag{2.54}$$

This will result in the same form as one obtains from the Weyl ordering of XP. Thus, in reality we do not really need any ordering prescription if we know the correct form of the star product. As mentioned before, we can imagine many different forms of quasi-probability distributions each with its own star product and as a consequence ordering prescription.

When performing practical calculations it is often useful to utilise the star product in the following form

$$(x^n \star p^m) \star a(x,p) = \left(x + \frac{i}{2}\frac{\partial}{\partial p}\right)^n \left(p - \frac{i}{2}\frac{\partial}{\partial x}\right)^m a(x,p) \tag{2.55}$$

which follows from Eq.(2.52) or Eq.(2.50). The differentials in Eq.(2.55) is called *Bopp operators* [14] or the representation of x and p in the *Bopp representation*

$$\hat{x} = x + \frac{1}{2}\frac{\partial}{\partial p}, \quad \hat{p} = p - \frac{1}{2}\frac{\partial}{\partial x}. \tag{2.56}$$

Changing the order of star-multiplication in Eq.(2.55) results in a change of the sign on the second term in both Bopp operators.

In the next section we will examine more closely the properties of the Wigner function that contains all the known information of our physical state.

2.4 Properties of the Wigner Function

Lets start by again stating the definition of the Wigner function expressed in terms of wave functions (in position space)

$$W(x,p) = \frac{1}{2\pi}\int \psi^*(x - \frac{1}{2}\tau)e^{-i\tau p}\psi(x + \frac{1}{2}\tau)d\tau. \tag{2.57}$$

It is easy to show that one has an equivalent definition for the Winger function in the momentum representation. Both these cases have the common idea that the state we examine is pure and is characterised by a vector $|\psi\rangle$. On the other hand, we can equally well consider a physical system that is formed from an ensemble of states, i.e. by a density matrix. The Wigner function is then generalised to

$$W(x,p) = \frac{1}{2\pi}\int \left\langle x - \frac{1}{2}\tau \middle| \hat{\rho} \middle| x + \frac{1}{2}\tau \right\rangle e^{-i\tau p}d\tau. \tag{2.58}$$

This form is the one we will study in this thesis. For the case $\hat{\rho} = |\psi\rangle\langle\psi|$ we re-obtain the original form Eq.(2.57).

2.4.1 Product of Wigner Functions: Overlap of States and Expectation Values

Before addressing the condition to be fulfilled in order fora function to be a probability distribution we first examine the language used in PSQM to express overlap between quantum states. We will find that it is directly connected to the trace formulation.

Suppose that we want to examine the product of two Wigner functions, corresponding to different density operators, integrated over phase space. What does the result represent? We start from the definition

$$2\pi \iint W_1(x,p)W_2(x,p)dxdp, \tag{2.59}$$

where the subscript indicate which density operator ,$\hat{\rho}_1$ or $\hat{\rho}_2$, the Wigner function is associated with. Explicitly this is

$$2\pi \iint W_1(x,p)W_2(x,p)dxdp = \iiint \tag{2.60}$$

$$\frac{1}{2\pi}\int e^{-i(\tau_1+\tau_2)p}\left\langle x+\frac{1}{2}\tau_1\right|\hat{\rho}\left|x-\frac{1}{2}\tau_1\right\rangle\left\langle x+\frac{1}{2}\tau_2\right|\hat{\rho}\left|x-\frac{1}{2}\tau_2\right\rangle dxd\tau_1 d\tau_2 dp. \tag{2.61}$$

Again using Eq.(2.36) and Eq.(2.37) this reduces to (setting $\tau = \tau_1 = -\tau_2$)

$$\iint \left\langle x+\frac{1}{2}\tau\right|\hat{\rho}\left|x-\frac{1}{2}\tau\right\rangle\left\langle x-\frac{1}{2}\tau\right|\hat{\rho}\left|x+\frac{1}{2}\tau\right\rangle dxd\tau \tag{2.62}$$

Making use of the completeness relation

$$\int dx' \left|x'\right\rangle\left\langle x'\right| = \mathbb{1} \tag{2.63}$$

and performing the change of variable to $x'' = x + \frac{1}{2}\tau$ and $x' = x - \frac{1}{2}\tau$ Eq.(2.62) finally becomes

$$2\pi \iint W_1(x,p)W_2(x,p)dxdp = \int dx'' \left\langle x''\right|\hat{\rho}_1\hat{\rho}_2\left|x''\right\rangle. \tag{2.64}$$

But this is nothing else then the definition of the trace operation over the product $\hat{\rho}_1\hat{\rho}_2$. Hence,

$$2\pi \iint W_1(x,p)W_2(x,p)dxdp = \mathrm{Tr}(\hat{\rho}_1\hat{\rho}_2). \tag{2.65}$$

This is a very important result. It allows us to make a direct connection to the extensive theory that exists about the density operator. For the expectation value we can calculate it in the same way as we did when we had a pure state but now we use the Wigner function corresponding to the density operator:

$$\mathrm{Tr}(\hat{\rho}A(X,P)) = \iint a(x,p)W_\rho(x,p)dxdp = \left\langle a(x,p)\right\rangle. \tag{2.66}$$

We see that the manner in which we calculate expectation values in phase space is the same regardless of whether the state is pure or mixed.

2.4.2 Condition on Probabiltiy Distrubtions

The Wigner function is not in every sense a true probability distribution as mentioned before. What do we mean when we say "true probability distribution"? Mathematically there are well defined properties a function has to satisfy to be called a probability distribution. Avoiding getting to bogged down with details we simply list two statements that we want a true probability distribution to satisfy, if any one of these two are does not hold we instead call the considered function a *quasi-probability distribution*:

$$1. \int f(x,p)dp = f(x), \qquad \int f(x,p)dx = \tilde{f}(p) \tag{Conditions}$$

$$2. f(x,p) \geq 0, \qquad \forall (x,p).$$

The first is usually called the *marginal condition*. It says that if we integrate over one of the variables we are left with the probability distribution for the other. This property is essential for practical calculations in the same way that $|\psi(x)|^2$ is (we will show in a moment that for the Wigner function they are the same thing). The second one is the property that the distribution function should not be negative for any combination of its function arguments. We call this the *positivity* condition. This is something that is always taken for granted when working with the classical theory; the concept of negative probability is nonsense in the classical physics where everything in principle is measurable. Yet, for a quantum mechanical system we will see that this is not always the case. The possibility for negative probability distributions are real in quantum mechanics and although shielded from direct observation, still constitute a vital part of the predictability power of the theory, as well as serving as a crucial part in our ability to visualise quantum states.

Let ut continue by showing that the Winger function reproduces the correct marginal distributions. Starting from Eq.(2.58) we integrate both sides with respect to p and rearrange the order of integration to obtain

$$\int W(x,p)dp = \frac{1}{2\pi} \int \left\langle x + \frac{1}{2}\tau \middle| \hat{\rho} \middle| x - \frac{1}{2}\tau \right\rangle d\tau \int e^{-i\tau p} dp. \tag{2.67}$$

Utilising the definition of the delta function, Eq.(2.36), along with the property stated in Eq.(2.37) we find

$$\int W(x,p)dp = \langle x| \hat{\rho} |x\rangle = W(x). \tag{2.68}$$

Thus, if we integrate the Wigner function with respect to the momentum variable p it yields the probability distribution in position space. For a pure state this reduces to

$$|\psi(x)|^2 = W(x), \tag{2.69}$$

which was hinted earlier. In addition this is in accordance with how we calculated the expectation value for an operator in Eq.(2.43) if the c-function $a(x)$ would only be a function of x, the result being identical to Eq.(2.12). To get the momentum marginal distribution we have to work a bit more but the result is the same, we obtain the probability distribution in momentum space (that is $|\tilde{\psi}(p)|^2$) [15].

For the second condition we utilise the trace formula, Eq.(2.65). We must have for two orthogonal density operators

$$\mathrm{Tr}(\hat{\rho}_1\hat{\rho}_2) = 0 = 2\pi \int dx \int W_1(x,p)W_2(x,p)dp, \tag{2.70}$$

which, provided the two Wigner function do not have compact support, implies that at least one of them cannot be positive definite (the case $W(x,p) = 0$ is clearly unphysical). The first statement can be made trivial true for a null density operator. Yet, for two non-zero orthogonal density operators, Eq.(2.70) is also true. We are thus forced to accept that in general it is possible for a Wigner function to take negative values. This violates the conditions stated before on complete positivity of a probability function. This is the reason why the Wigner function is called a quasi-probability distribution, for a general state it is not strictly positive [14]. The reason for this shortcoming has its root in the foundation of quantum theory. As mentioned before it is possible to construct an infinite number of distribution functions that capture quantum mechanics. None of them will be able to pass every test that is required to be a true probability distribution (these includes additional conditions that we did not list). Nevertheless, they are still extremely useful and capture fully the physical state.

2.4.3 Bounded Condition on The Wigner Function

One of the most common objection when one is introduced to the PSQM is that it does not respect the uncertainty principle between position and momentum. That in principle we could shrink the Wigner function to a single point with defined coordinates (x,p) and thus we would know its position and momentum exactly. It turns out however that the Wigner function can not take on arbitrary small values (or large for that matter). In other words, the Wigner function is *bounded.* To start, we can see that the

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[14] It is sometime stated by some authors that the ability for the Wigner function to be negative capture by itself all of the strangeness of quantum mechanics. This is a symptom of poor understanding. The distrubtion function and its properties are only one of the defining properties of quantum mechanics in phase space. In fact there are states (all variations of the ground state of the harmonic oscillator) which results in strictly positive Wigners functions. These are of course still quantum mechanical states.

condition

$$\mathrm{Tr}(\hat{\rho}^2) \leq 1 \tag{2.71}$$

on the density operator translate to the condition on the square of the Wigner function in the way that

$$2\pi \leq \frac{1}{\int dx \int W^2(x,p)dp}. \tag{2.72}$$

It can be shown [15] that the right hand side corresponds to an area in phase space. The equality only holds for a pure state. This result then tells us that the Wigner function can never occupy an arena smaller than 2π. It is also possible to explore the smallest and largest numerical value the Wigner function can take.

Starting from the definition Eq.(2.57) for the Wigner function of a pure state (expressed in terms of the wave-functions) we can reinterpret this by defining two new normalised wave-functions in the following way

$$\phi_1(\tau) = \frac{1}{\sqrt{2}} e^{ip\tau} \psi(x - \frac{1}{2}\tau) \qquad \text{and} \qquad \phi_2(\tau) = \frac{1}{\sqrt{2}} \psi(x + \frac{1}{2}\tau) \tag{2.73}$$

with this Eq.(2.57) can be expressed as

$$W(x,p) = \frac{1}{\pi} \int \phi_1^*(\tau) \phi_2(\tau) d\tau, \tag{2.74}$$

but ϕ_1 and ϕ_2 are the wave-functions in the τ representation such as $\phi_1^* = \langle \phi_1 | \tau \rangle$, therefore

$$W(x,p) = \frac{1}{\pi} \int \phi_1^*(\tau) \phi_2(\tau) d\tau = \frac{1}{\pi} \langle \phi_1 | \phi_2 \rangle \tag{2.75}$$

where we have used the completeness relation for τ ($\int |\tau\rangle \langle \tau| = \mathbb{1}$). We are now in the position to use the Cauchy-Schwarz inequality. Applied to our case we have

$$|\langle \phi_1 | \phi_2 \rangle|^2 \leq \langle \phi_1 | \phi_1 \rangle \cdot \langle \phi_2 | \phi_2 \rangle = 1 \cdot 1 \tag{2.76}$$

since the states $|\phi_1\rangle$ and $|\phi_2\rangle$ are normalised. This then constrains the Wigner function

$$-\frac{1}{\pi} \leq W(x,p) \leq \frac{1}{\pi}. \tag{2.77}$$

Thus, the Wigner function cannot take arbitrary large or small values. The condition on smallest area from above prevents us from shrinking the phase space distribution in such a way that we can determine exactly both the position and momentum. This is one of the ways in which the uncertainty principle manifests itself in PSQM[15].

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[15] There is actually an equivalent way to state the uncertainty principle in PSQM to the ordinary one, where one instead use the star product discussed earlier to make the corresponding statement.

2.4.4 Time Evolution for The Wigner Function

Up till now we have suppressed the time dependence of the Wigner function. From the defining equation Eq.(2.58) we see, however, that if the density operator have a time dependence then so too does the Wigner function. The question then is how can we obtain an equation of motion for the Wigner function? There is two ways we can go about this. Either we exploit the fact that the density operator satisfy a well known equation of motion, or alternatively, we follow the path of Moyal and define an infinitesimal kernel that induces time-evolution [13]. The second alternative is interesting in the way that it does not give a reference to the operator formalism. Yet, the first one is the more direct approach and is also a prime candidate to use of some of our techniques developed earlier in section 2.3.

The density operator satisfy the *von Neumann* equation of motion [10]

$$\frac{\partial \hat{\rho}}{\partial t} = \frac{1}{i}[\hat{H}, \hat{\rho}]. \tag{2.78}$$

We now want to transfer this equation to phase space. This is lissom done by noting that we already know how each object is represented in phase space. The correspondence for the density operator is just our well known Wigner function. For the Hamiltonian correspondence we would image that we be forced to tread a bit careful as we many explicit forms are possible [16]. Per contra we already possess a general scheme for converting any general operator to phase space by the Weyl ordering. With that said, the most common and simple form of the Hamiltonian $\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{x})$ is converted by just replacing operators with classical variables p and x. Finally we convert the commutator between $H(x,p)$ and $W(x,p)$ to the Moyal bracket discussed in section 2.3.5. Hence, our equation of motion for the Wigner function reads

$$\frac{\partial W(x,p;t)}{\partial t} = \frac{1}{i}\{H(x,p), W(x,p;t)\}_{MB}. \tag{2.79}$$

If instead we choose to derive this as Moyal we would of course obtain the same result. For time-independent pure state Wigner functions we can formulate eigenvalue equations akin to those in conventional Schrödinger quantum mechanics by using the star product. We will sadly not have any opportunity to use those so we will not explore that subject in any detail[17]. We close this section by pointing out the similarity between Eq.(2.79) and the classical *Liouville's theorem*. The relation to the classical theory will be discussed in the next section.

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[16] We have ignored the possibility of spin here, more on that later.

[17] This aspect is however very important for the general formulation of the theory of PSQM.

2.4.5 Connection to The Classical Theory and A Remark on Units

Up till this section we have worked in units where $\hbar = 1$. This is done to simplify notation to more clearly bring out the framework of the theory. Yet, we still have to know where to put in the appropriate constants to give our expectation value the correct dimension of units. Furthermore, it is known that the connection to classical mechanics is often retrieved in the limit $\hbar \to 0$ [8] (sometime called the *Correspondence principle*[6]). In none of the formulations of quantum mechanics is this fact more clearly illustrated then in the PSQM. Before exploring how our previously derived results depend on $\hbar$ we quickly point out that to make sense of units when dealing with operators we have to assign units to these operators in addition to constants and functions.

We will now restate results from previous sections and discus their classical limit:

- There are several equivalent ways to state the Wigner function when one includes $\hbar$ depending on how one defines the Fourier transform variable (we called it τ). The most direct way to see the classical limit is if we define the Wigner function (for a pure state) as

$$W(x,p) = \frac{1}{2\pi}\int \psi^*(x - \frac{1}{2}\tau\hbar)e^{-i\tau p}\psi(x + \frac{1}{2}\tau\hbar)d\tau. \tag{2.80}$$

  We note that the limit $\hbar \to 0$ results in a perfectly determined probability distribution in x-space times a δ function in p-space. The Wigner function transforms in the classical limit to a true probability distribution which always is positive and still satisfy the marginal conditions. This is exactly what we would suspect from any classical theory. The Wigner function for a given density operator reads

$$W(x.p) = \frac{1}{2\pi}\int e^{-i\tau p}\left\langle x + \frac{1}{2}\tau\hbar\middle|\, \hat{\rho}\, \middle| x - \frac{1}{2}\tau\hbar\right\rangle d\tau. \tag{2.81}$$

- The bounds of the Wigner function go to infinity in the classical limit. We can see this from the result in Eq.(2.77) if we include $\hbar$ (this stem from the definition of the Wigner function if we make the substitution $\tau' = \tau\hbar$)

$$-\frac{1}{\pi\hbar} \leq W(x,p) \leq \frac{1}{\pi\hbar}. \tag{2.82}$$

  In the classical limit the Wigner function is allowed to take on arbitrary large (or small non-negative) values.

- If we instead define the Fourier transform variable in a different way we will, for example, get that the $\hbar$ dependence of the star product between two c-functions

  $$\star = e^{\frac{i\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)} \tag{2.83}$$

  which is of vital importance in Moyals equation Eq.(2.79)

  $$\frac{\partial W(x,p;t)}{\partial t} = \frac{1}{i\hbar}\{H(x,p), W(x,p;t)\}_{MB}. \tag{2.84}$$

  If we expand the star product between $H(x,p)$ and $W(x,p)$ we find that

  $$\begin{aligned} \frac{\partial W(x,p;t)}{\partial t} &= \{H(x,p), W(x,p;t)\}_{PB} \\ +H(x,p) \sum_{k=2}^{\infty} &\left(\frac{i\hbar}{2}\right)^k \frac{1}{k!} \left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)^k W(x,p) \\ -W(x,p) \sum_{k=2}^{\infty} &\left(\frac{i\hbar}{2}\right)^k \frac{1}{k!} \left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)^k H(x,p), \end{aligned} \tag{2.85}$$

  where $\{...\}_{PB}$ is the *Poisson bracket* [16] from classical mechanics. Thus, the equation of motion for the Wigner function is the same as for a classical phase space distribution[18] plus quantum corrections. We will later see that this naturally emerges when one performs calculations to obtain the equations of motion. One usually arrive with a term that is purely classical in addition to terms that are quantum corrections to that as seen in Eq.(2.85) as the expansion in powers of $\hbar$. In this way we can reap the benefit of PSQM, by working with a form which is often easier to analyse from a physical point of view. In addition, as we will see in this thesis, for certain models the expansion Eq.(2.85) terminates already for some low powers of $\hbar$. Moreover this can be used to carry out first approximation calculations by first calculating the result for the classical terms ("classical trajectory") and then adding quantum fluctuations to that trajectory. Again we also have that when taking the limit $\hbar \to 0$ we recover the classical equations of motion. In the language of deformation quantization, the Moyal bracket is just the deformation of the Poisson brackets from classical mechanics.

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[18] The classical analogy to Eq.(2.79) is *Liouville's equation* $\frac{\partial}{\partial t} f(x,p;t) = -\{H(x,p), f(x,p;t)\}_{PB}$ which describes the time-evolution of a classical phase space distribution.

2.5 Interlude: Coherent States

In this section we summarise the theory and results concerning coherent states and the creation and annihilation operators [10][6]. We will need this for defining another quasi-probability distribution; the *Husimi function* denoted by the Q symbol [15]. This discussion is in no manner exhaustive.

2.5.1 Canonical Coherent States

Coherent states most common appearer when one studies the quantum harmonic oscillator (QHO) characterised by the Hamiltonian

$$\hat{H} = \frac{\omega}{2}(\hat{x}^2 + \hat{p}^2) \tag{2.86}$$

with $\hat{x}$ and $\hat{p}$ rescaled to make the expressions more symmetrical, and also more directly connected to the field quadratures of any general boson field [17]. A frequent procedure for solving the QHO is to introduce the non-hermitian operators

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{p}) \qquad \text{and} \qquad \hat{a} = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{p}) \tag{2.87}$$

called the *creation* and *annihilation operators* (or *ladder operators* together). The QHO Hamiltonian then reads

$$\hat{H} = \omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}\hat{\mathbb{1}}) \tag{2.88}$$

and the known commutator relations for $\hat{x}$ and $\hat{p}$ is converted to the commutator relations for $\hat{a}$ and $\hat{a}^\dagger$

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{2.89}$$

Working in this framework it becomes especially simple to solve the QHO problem, i.e. finding the eigenstates and the corresponding energies. It i,s however, the ground-state that is of interest for us. The QHO ground-state is namely a minimum uncertainty state, meaning that it satisfies the equality in the uncertainty principle [10]. As it turns out, the key result that leads to this is the action of the annihilation operator on the ground-state (the vacuum state) $\hat{a}\,|0\rangle = 0\,|0\rangle = 0$. Inspired by this we ask the question: Is there any state which when acted on by $\hat{a}$ remains unchanged? Formulated in mathematical terms

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle\,, \tag{2.90}$$

where α can be a complex number since $\hat{a}$ is not a hermitian operator and $|\alpha\rangle$ is the proposed eigenstate to $\hat{a}$. We also note that the hermitian conjugate of this statement is

$$\langle\alpha|\,\hat{a}^\dagger = \alpha^*\,\langle\alpha|\,. \tag{2.91}$$

To check if this is a valid proposition we calculate the variances of $\hat{x}$ and $\hat{p}$ in the state $|\alpha\rangle$. Working with the dimensionless parameters (scale the energy $\hat{H}/\omega$) we have

$$\langle\alpha|\,\hat{x}^2\,|\alpha\rangle = \frac{1}{2}\,\langle\alpha|\,(\hat{a}^\dagger + \hat{a})^2\,|\alpha\rangle = \frac{1}{2}(\alpha+\alpha^*)^2 + \frac{1}{2}, \tag{2.92}$$

which readily follows from Eq.(2.89), Eq.(2.90) and Eq.(2.91). In the same way we can calculate the variance of $\hat{p}^2$

$$\langle\alpha|\,\hat{p}^2\,|\alpha\rangle = \frac{1}{2}\,\langle\alpha|\,(\hat{a}^\dagger - \hat{a})^2\,|\alpha\rangle = \frac{1}{2}(\alpha-\alpha^*)^2 - \frac{1}{2}. \tag{2.93}$$

The variance is defined as the difference between the expectation value of the square minus the expectation value squared

$$\langle(\Delta\hat{x})^2\rangle_\alpha = \langle\hat{x}^2\rangle_\alpha - \langle\hat{x}\rangle_\alpha^2 = \frac{1}{2} \tag{2.94}$$

(which follows from $\langle\alpha|\,\hat{x}\,|\alpha\rangle) = \frac{1}{\sqrt{2}}(\alpha+\alpha^*)$). Identically we get

$$\langle(\Delta\hat{p})^2\rangle_\alpha = \frac{1}{2}. \tag{2.95}$$

Hence,

$$\langle(\Delta\hat{x})^2\rangle_\alpha \cdot \langle(\Delta\hat{p})^2\rangle_\alpha = \frac{1}{4} \tag{2.96}$$

which is the lower bound of the uncertainty principle. Thus, there should exist other states except the ground-state of the QHO that are minimum-uncertainty states. These states $|\alpha\rangle$ are called *coherent states* (or *canonical coherent states* to separate them from other kinds of coherent states).

The coherent states expressed in the number basis read [10]

$$|\alpha\rangle = e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}(\hat{a}^\dagger)^n\,|0\rangle\,, \tag{2.97}$$

from which it follows that the photon distribution $P(n) = |\langle n|\alpha\rangle|^2$ is Poissonian. This can also be rewritten if we note that the right hand side is just the expansion of an exponential containing $\hat{a}^\dagger$

$$|\alpha\rangle = e^{-|\alpha|^2/2}e^{\alpha\hat{a}^\dagger}\,|0\rangle\,, \tag{2.98}$$

which can be alternatively expressed by inserting $e^{-\alpha^*\hat{a}}$ to the left of the vacuum state. This is possible because of the expansion of the exponential will result in a factor 1 since $\hat{a}$ annihilates the vacuum state. Thus,

$$|\alpha\rangle = e^{-|\alpha|^2/2}e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}\,|0\rangle = e^{\alpha\hat{a}^\dagger-\alpha^*\hat{a}}\,|0\rangle = \hat{D}(\alpha)\,|0\rangle \tag{2.99}$$

where we made use of the Baker-Hausdorff theorem and in the last line defined the *displacement operator* $\hat{D}(\alpha)$. Hence, we can obtain a coherent state by acting on the vacuum state with the displacement operator. Indeed, by using the Baker-Hausdorff theorem it follows that the displacement operator acting on any coherent state results in a new coherent state, and thereby the name "displacement". It can be shown [15] that the coherent states constitute an *over-complete* base with the closure relation

$$\hat{\mathbb{1}} = \frac{1}{\pi} \int d^2\alpha \, |\alpha\rangle \langle\alpha| \,, \tag{2.100}$$

where the over-completeness appears in the extra factor of π.

It is possible to express the Wigner function as a function of α and α^* by using Eq.(2.87) to replace $\hat{x}$ and $\hat{p}$ with $\hat{a}^\dagger$ and $\hat{a}$. All other results derived in previous sections can also straightforwardly be generalise to this basis. An alternative phase space representation in the complex parameter α is the Husimi Q-function discussed in section 2.6. As we will see, the over-completeness Eq.(2.100) turns out to be crucial for the Husimi function.

2.5.2 Spin Coherent States

The construction and features of *spin coherent states* are slightly more complicated than those for the canonical coherent states. This derives from the space in which the states live; spins live on a sphere meaning that the space is not flat, and furthermore it is compact. We will simply state the necessary definitions and relations. The interested reader is referred to [18][19] .

We define the ladder operators for angular momentum as

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y \tag{2.101}$$

which satisfy the commutator relations

$$\begin{aligned} [\hat{J}_3, \hat{J}_\pm] &= \pm\hat{J}_\pm \\ [\hat{J}_+, \hat{J}_-] &= \hat{J}_3 \end{aligned} \tag{2.102}$$

and when acting on a state characterised by the quantum numbers m (eigenvalue to the spin in z-direction) and j (related to the eigenvalue of $\hat{J}^2$) results in [10]

$$\hat{J}_+ |j, m\rangle = \sqrt{(j-m)(j+m+1)} \, |j, m+1\rangle \,, \tag{2.103}$$

$$\hat{J}_- |j, m\rangle = \sqrt{(j+m)(j-m+1)} \, |j, m-1\rangle \,. \tag{2.104}$$

Thus, the effect of the ladder operators is to raise or lower the value of m by one. We also note that this implies that

$$\hat{J}_+ \left|j, j\right\rangle = 0 \tag{2.105}$$

for a maximum weight state where $m = j$, and

$$\hat{J}_- \left|j, -j\right\rangle = 0 \tag{2.106}$$

for a minimum weight state where $m = -j$.

The analogue to the displacement operator is the *Bloch rotation operator*

$$R(z) = N e^{z\hat{J}_-} e^{\ln\left(1+|z|^2\right)\hat{J}_z} e^{-z^*\hat{J}_+} \tag{2.107}$$

with $z = \tan\left(\frac{\theta}{2}\right)e^{i\phi}$ (the angle variables θ and ϕ refer to Euler angles for the *Bloch sphere*[19]) and N a normalisation factor. .When acting on the extremal state (could be either the highest or lowest level of spin) of angular momentum $\left|j, j\right\rangle$ with $R(z)$ this produce a *spin coherent state*

$$\begin{aligned} \left|z\right\rangle = N e^{z\hat{J}_-} e^{\ln\left(1+|z|^2\right)\hat{J}_z} e^{-z^*\hat{J}_+} \left|j, j\right\rangle &= N e^{z\hat{J}_-} e^{\ln\left(1+|z|^2\right)\hat{J}_z} \left|j, j\right\rangle \\ &= N' e^{z\hat{J}_-} \left|j, j\right\rangle , \end{aligned} \tag{2.108}$$

where we used the fact that $\hat{J}_+$ acting on $\left|j, j\right\rangle$ is zero, and that $e^{\ln\left(1+|z|^2\right)\hat{J}_z} \left|j, j\right\rangle = e^{\ln\left(1+|z|^2\right)j} \left|j, j\right\rangle$ and including it in the new definition of N'. The normalisation constant can be determined by examining the effect of ladder operators acting on $\left|z\right\rangle$. Our final form for the *spin coherent state* is

$$\left|z\right\rangle = \frac{1}{(1+|z|^2)^j} e^{z\hat{J}_-} \left|j, j\right\rangle . \tag{2.109}$$

By performing some cumbersome calculations it can be shown that the resolution of unity takes the form

$$\int \left|z\right\rangle \left\langle z\right| \frac{2j+1}{\pi} \frac{d^2 z}{(1+|z|^2)^2} = \mathbb{1}. \tag{2.110}$$

The spin coherent states are in the same way as canonical coherent states, states that minimise the uncertainty relation. One caveat is that not all spin coherent states can satisfy the minimum uncertainty relation at the same time. This is in contrast to the canonical coherent states which does not obey such a restriction.

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[19] The Bloch sphere is a representation of a spin state. Arbitrary spin can then be represented by a point on or inside the sphere.

2.6 The Husimi Function

Aside from the Wigner function we will study one more quantum mechanical quasi-probability distribution in this thesis. In principle there is no need for another distribution besides the Wigner function, since, as we have stated many times, the Wigner function contains all the physical information of our system. Yet, there is advantages to introduce other quasi-probability distributions. We will see that the Husimi function have the neat property of being positive definite, in contrast to the Wigner function. In addition it is defined by referring directly to coherent states. Lastly, the ordering process when going from quantum mechanical operators to a c-function is simple in its realisation when expressed with the creation and annihilation operators.

In order to define the Husimi function we will follow a different approach compared to the one used when introducing the Wigner function. We start by asking the question what distribution corresponds to *anti-normal* ordering of an arbitrary collection of creation and annihilation operators? Recall that anti-normal ordering is when every creation operator is to the right of the annihilation operators. If we consider a operator (polynomial) that is a function of $\hat{a}$ and $\hat{a}^\dagger$ it can be expressed with this ordering prescription as

$$\hat{A}(\hat{a}, \hat{a}^\dagger) = \sum_{m,n=0}^{\infty} d_{m,n} \hat{a}^m (\hat{a}^\dagger)^n, \tag{2.111}$$

where $d_{m,n}$ are the coefficient of the expansion. This form can always be obtained by reordering arbitrary operator by using the commutator relations for $\hat{a}$ and $\hat{a}^\dagger$. A particular operator that satisfy this ordering procedure is

$$\hat{A}(\hat{a}, \hat{a}^\dagger) = e^{-\lambda^* \hat{a}} e^{\lambda \hat{a}^\dagger}, \tag{2.112}$$

which can be seen by expanding the exponentials. To be of any use to us we should be able to calculate the expectation value of an operator ordered in this way with a certain probability distribution. We can choose the following representation of the density operator

$$\hat{\rho} = \int P(\alpha) \left|\alpha\right\rangle \left\langle\alpha\right| d^2\alpha \tag{2.113}$$

which follows from the completeness relation for the canonical coherent states, Eq.(2.100), and the general form of the density operator $\hat{\rho} = \left|\psi\right\rangle \left\langle\psi\right|$. In Eq.(2.113), $P(\alpha)$ is a general distribution function (not a probability distribution!) that give a measurement of the distribution of coherent states in the complex phase space spanned by α and α^*. In the literature it is called *the Glauber-Sudarshan P-distribution* and is used to calculate other forms of expectation values[20]. With this we calculate the expectation value of the particular form of the operator A as given above in the usual fashion

$$\left\langle \hat{A}(\hat{a},\hat{a}^\dagger)\right\rangle = \int P(\alpha)\left\langle\alpha\right|\hat{A}\left|\alpha\right\rangle d^2\alpha = \mathrm{Tr}[\hat{\rho}\hat{A}] = \mathrm{Tr}[\hat{\rho}e^{-\lambda^*\hat{a}}e^{\lambda\hat{a}^\dagger}] \tag{2.114}$$

inserting the completeness relation for the coherent states Eq.(2.100) and remembering the cyclic property related to the trace action we can write this as

$$\mathrm{Tr}[\hat{\rho}e^{-\lambda^*\hat{a}}e^{\lambda\hat{a}^\dagger}] = \mathrm{Tr}\left[\hat{\rho}e^{-\lambda^*\hat{a}}\left(\frac{1}{\pi}\int\left|\alpha\right\rangle\left\langle\alpha\right| d^2\alpha\right)e^{\lambda\hat{a}^\dagger}\right]. \tag{2.115}$$

Recalling the eigenvalue equations for $\hat{a}$ and $\hat{a}^\dagger$:

$$\langle A\rangle = \frac{1}{\pi}\int e^{\lambda\alpha^*-\lambda^*\alpha}\left\langle\alpha\right|\hat{\rho}\left|\alpha\right\rangle d^2\alpha = \int a(\alpha,\alpha^*)Q(\alpha,\alpha^*)d^2\alpha, \tag{2.116}$$

where we have defined the c-function $a(\alpha,\alpha^*) = e^{\lambda\alpha^*-\lambda^*\alpha}$ corresponding to $\hat{A}(\hat{a},\hat{a}^\dagger) = e^{-\lambda^*\hat{a}}e^{\lambda\hat{a}^\dagger}$ and the quasi-probability distribution

$$Q(\alpha,\alpha^*) = \frac{1}{\pi}\left\langle\alpha\right|\hat{\rho}\left|\alpha\right\rangle \tag{2.117}$$

called the *Husimi function* (or the *Q-function*). We have achieved our goal of finding a quasi-probability distribution that allows us to calculate expectation values of operators which are anti-normally ordered. The Q-function is simply the expectation value of the density operator in coherent states. In addition it is easy to see that in contrast to the Wigner function, the Husimi function is always positive. If we in Eq.(2.117) insert the density operator on the form $\sum_i \hat{\rho}_i = \left|\psi_i\right\rangle\left\langle\psi_i\right|$ and recall that $|\left\langle\psi_i|\alpha\right\rangle|^2 \geq 0$ for every i the result follows

$$Q(\alpha,\alpha^*) = \sum_i \frac{1}{\pi}|\left\langle\psi_i|\alpha\right\rangle|^2 \geq 0, \tag{2.118}$$

therefore we are working with a always positive function. This can be used to ease the visualisation of states in phase space when negative areas may seem odd at first sight. On the other hand, we can clearly see from Eq.(2.117) that $Q(\alpha,\alpha^*)$ can not

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[20] The $P(\alpha)$ distribution is connected to the Q-function in the way that it is the diagonal representation of the density operator when taken in between coherent states. It is used when expectation values of an operator that is normal-ordered is desired. It however suffered from displaying not so nice symptoms like singular functions and is not something that we will use any further in this thesis except as a tool for obtaining the Q-function.

satisfy the marginal condition stated in section 2.4.2. That is, we cannot integrate over one variable to obtain the corresponding probability distribution for the remaining one. We are still working with a quasi-probability distribution with some form of shortcoming[21]. It is interesting to note that the Husimi function $Q(\alpha, \alpha^*)$ is simply the diagonal elements of the density operator in the basis of coherent states. At first this seems as contradicting the fact that any information about the state is contained in $Q(\alpha, \alpha^*)$; the off-diagonal terms should also contain some information. The "magic" behind this is hidden in the fact that the coherent states form an over-complete basis. The sacrifice is the failure of the marginal condition which in a sense is a indication on how "accessible" the information is. In addition, the star-product (and the resulting equation of motion) will also differ from the Wigner-case, and information that was though lost are now present there instead (in the form of a more complicated star-product) when considering the dynamic.

The connection to the Wigner function can be established by using a more general framework then that developed in section 2.3. This generalisation is not especially more difficult and the interested reader is refereed to [7].

We close this section by noting that the time-evolution equation for the Q-function can be obtained in the same manner as for the Wigner function. Starting from the von Neumann equation of motion one multiply both sides by $\langle\alpha|$ from the left and by $|\alpha\rangle$ from the right. In the calculation part we will see a concrete example of this.

2.7 Spin in The Phase Space Formulation of Quantum Mechanics

Up until this point we have exclusively considered a system where the only dynamical degrees of freedom consist of position and momenta. Yet, to be a fully functional formulation of quantum mechanics we have to be able to capture every conceivable property directly in phase space. The hallmark feature that is most striking that we have omit is of course *spin* (and the resulting distinction between bosons and fermions). This intrinsic property of a particle is a defining trait of quantum mechanics and lack any classical counterpart. All hope of relating spin to classical mechanics is however not lost completely as spin behaves as a sort of angular momenta.

The natural question is then how to repeat the previous construction of the framework in a way that is also valid for spin? From a fundamental point of view we have two options. Either we extend our current framework to include spin, or we can modify

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[21] For the Wigner function the possibility for negative values was however an asset that could indicate quantum interference while the failure for the Husimi function to capture the marginal condition do not have any apparent advantage.

our approach in such a way that the final construction can handle both position and momenta as well as spin. In the end, the result must in both cases be the same, a fully developed theory that can describe spin in all its glory. Sadly, it turns out that the construction of a theory for spin is unfortunately a complicated story in the PSQM. This can be traced back to at least two points which are related. Firstly, we know from the operator formulation of quantum theory that the operators corresponding to spin do not satisfy a canonical commutation relation, but instead fails to commute in a way which is characterised by [10]

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k \tag{2.119}$$

with i, j, k corresponding to the three spatial-dimensions and where ϵ_{ijk} is the *Levi-Civita symbol.* Eq.(2.119) is drastically different from the canonical commutation relation[22] in the way that we now have on the right hand side an operator as a measurement on the failure of commutation amongst the spin operators for each direction. The consequence of this is maybe not that apparent on a first inspection but are nevertheless dramatic. Secondly, related to this fact, is something that we already encountered preciously, albeit only in passing. When we discussed spin coherent state in section 2.5.2 we mentioned that the spin is parametrised on a sphere, known as the Bloch sphere. An analogy to this is the Poincaré sphere which exist in classical optics where it represents polarisation. As a consequence of this we can expect that the phase space where spin lives is not a flat surface as before but instead the surface of a sphere. This change of geometry from flat to curved geometry forces us to modify (or generalise) how we relate operators to phase space functions.

There exist at least three ways for describing and treating spin. Of these, two can be considered more rigorous. We will not discuss any of these methods in detail because that would require techniques that is outside the scope of this thesis.

2.7.1 Method 1: Schwinger Spin Representation

The first method can be considered the most straightforward but also the one which is the least rigorous as it relies on assumptions imposed on the system[23]. It is known from the operator formalism of quantum mechanics that spin can be represented by two coupled oscillators [10], this is known as the *Schwinger representation of spin* (or angular momentum). By exploiting this fact we can extend our formalism in a direct

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[22] The same can be said about its classical counterpart, the Poisson bracket for angular momentum [16] which is different then that between position and momenta.

[23] For example the number of "spin" bosons have to be conserved to ensure the correspondence between the harmonic oscillator and spin algebra.

manner without worrying about any explicit spin dependence. What are the disadvantages of this method? Aside from requiring us to tread carefully when examining the detail structure of a system (as this representation is only strictly true for spin 1/2 particles) it also introduce extra variables which in the end have to be eliminated to minimise the already present computational complexity. In other words, we introduce more variables then should be needed to characterise the system. In addition, this method quickly result in overwhelming calculations when a large amount of spin terms are present.

2.7.2 Method 2: The Stratonovich-Weyl Correspondence

The second method constitutes a generalisation of our previous arguments used in this chapter. In its essence, the method imposes mathematical and physical properties on the map between operators and phase space functions that must be satisfied in order to arrive at a physically sound formalism. This procedure is known as the *Stratonovich-Weyl correspondence* [20, 21] and is valid for any geometry , thus it can be considered as the most general formulation of PSQM. In practice, this method is however cumbersome to deal with. This can again be traced back to the complicated geometry needed to describe spin (compared to the previous flat case). For example, the need of spherical harmonics and Casimir operators are required in order to describe the spin. The resulting star-product between spin functions is discouraging to say the least. For the mathematically trained researcher this method can maybe be considered usable, but even then only for simple systems.

2.7.3 Method 3: Grassmann Variable Quantization

The third and last method that can be found in use are based on *Grassmann variables* [20, 22, 23]. This method is akin to the path integral formulation for fermions, well known in quantum field theory, where it arouse out of the need for a classical counterpart to fermionic fields [24]. The basic idea is the same in the PSQM, Grassmann variables are introduced as a classical concept and then quantized with an appropriate star-product. Utilising this we can describe systems containing fermions [23]. With this all results follows in a similar way as before, only now we have in addition to ordinary numbers a new type of numbers that anti-commute. This method is however a bit misleading as the presence of Grassmann variables do result in some complications which are not directly apparent. Aside from the complication of physical interpretation caused by Grassmann variables we also encounter a more severe problem. The most prominent is the loss of clearly defined integration operation. For Grassmann variables, integration is defined purely algebraically [23], this can cause problem when, for example, calculating the marginal probability from the Wigner function.

3 Open Quantum Systems

In this section we will discuss the necessary features of open quantum systems that we will need later on in this thesis. The field of open quantum systems are a large and interesting area of research and we cannot hope to even cover a small part of the existing framework. At the heart of treating open systems is the concept of stochastic processes that conveys the effect of the connection of an isolated system to an environment. This proposition to split a total quantum system into an environment and a system to be investigated is central to the study of open systems. Thus, an open quantum system is one where we can split the total system into two parts. One we call, as already mentioned, the *environment* and is often assumed to be the larger of the two parts (contains more degrees of freedom). In addition we are usually not interested in the dynamic of the environment, which by itself many times would be almost impossible to obtain in any case as a consequence of its vast size. This is the chief reasons for splitting the original total quantum system into two parts. The other part is what we denote the *system* (or system of interest). For this distinction to be true we must in addition have a weak coupling strength between the system and the environment. With this we mean that the relevant time-scale of the system are short relative the system-environment interaction time-scale. Hence, the coupling is weak compared when measured against other time-scales. The system part dynamics will not be the same as if it was isolated but will instead be influenced by the environment. It is this coupling between the system and the environment that give rise to to the effect of *decoherence.*

We will examine an important dynamical equation that governs the time-evolution of the systems density operator. This is obtained by first starting from a very general form. However, it is not possible to obtain a general equation describing any interaction of the system with a general environment. Yet, by invoking physical gumptions (sound) approximations we can in fact obtain a rather general equation of motion for the system, i.e a master equation.

The layout of this section is as follows. First we mention the broad concept of partial trace and how this is used to obtain the density operator for the system alone. After that we start our derivation of what will be known as the *Born-Markov master equation*, the equation that describes how the system density operator evolves in time when under the influence of interaction with the environment. After this we consider some specific cases which are of interest to us in this thesis. We end with a short discussion on decoherence and how it is related to the dynamics of open quantum systems.

3.1 Reduced Density Operator by Partial Trace

As already mentioned several times before, the density operator contains all physical information about the considered system. We now want to derive an expression for a reduced density operator that describe only a part of the total system. When the full system state does not show correlations between its two constituent parts, system plus environment, we have

$$|x_S, y_E\rangle = |x_S\rangle \otimes |y_E\rangle \,, \tag{3.1}$$

where x_S is the degrees of freedom associated with the system, and y_E the degrees of freedom associated with the environment. Eq.(3.1) is a *pure state* which does not exhibit any entanglement. This is not a flawed assumption as we can always consider such a large quantum system that it by itself is isolated (the entire universe) and thus can be considered a state which can leads itself to one configuration, a pure state. Moreover, the time-evolution is unitary as the total system can be considered isolated (this is not true for sub-parts of a total system). We will however see that the parts of the global system must be described by density operators and hence are necessarily mixed states. This restriction is not present when discussing the state for the total system which can be described as a pure state (or in general also by a density matrix).

With Eq.(3.1) we can now consider operators which only act on the system and on the environment separately (or by a unitary action on the non- referred part). If we want to, for example, calculate the expectation value of an operator only defined on the system degrees of freedom (system space) we have

$$\langle x_S, y_E| \hat{A} |x_S, y_E\rangle = \langle x'_S| \otimes \langle y'_E| \hat{A} |x_S\rangle \otimes |y_E\rangle = \delta_{y'y} \langle x'_S| \hat{A} |x_S\rangle \,, \tag{3.2}$$

where in the last step we assumed that the environment states are orthonormal to each other. Proceeding further with this example we instead consider the expectation value of the operator $\hat{A}$ taken with respect to any quantum state $|\psi\rangle$

$$\langle\psi| \hat{A} |\psi\rangle = \sum_{xx'} \sum_{yy'} \langle\psi|x_S, y_E\rangle \langle x_S, y_E| \hat{A} |x'_S, y'_E\rangle \langle x'_S, y'_E|\psi\rangle \tag{3.3}$$

where we inserted the completeness relation for $|x_S, y_E\rangle$ twice. From Eq.(3.2) we know how to express the matrix element of $\hat{A}$. Thus we can write $\langle\psi| \hat{A} |\psi\rangle$ as

$$\begin{gathered}\sum_{xx'} \sum_{yy'} \langle\psi|x_S, y_E\rangle \, \delta_{y'y} \langle x_S| \hat{A} |x'_S\rangle \langle x'_S, y'_E|\psi\rangle = \\ \sum_{xx'} \sum_{y} \langle\psi|x_S, y_E\rangle \langle x_S| \hat{A} |x'_S\rangle \langle x'_S, y'_E|\psi\rangle = \mathrm{Tr}_S(\rho_S \hat{A})\end{gathered} \tag{3.4}$$

with

$$
\begin{aligned}
\rho_S = \sum_{xx'}\sum_{y} |x'_S\rangle \langle x'_S, y_E|\psi\rangle \langle\psi|x_S, y_E\rangle \langle x_S| = \\
\sum_{xx'}\sum_{y} |x'_S\rangle (\langle x'_S| \langle y_E|) |\psi\rangle \langle\psi| (|y_E\rangle |x_S\rangle) \langle x_S| = \\
\mathrm{Tr}_E(|\psi\rangle\langle\psi|) = \mathrm{Tr}_E(\rho_{total})
\end{aligned}
\tag{3.5}
$$

which is the *reduced density operator* describing the system S. We see that by taking the trace over the environment variables we obtain a density operator which only describes the system and we can use it to calculate expectation values of operators acting only in the system space. Furthermore, we note that the total system was described by a pure state but parts of the system is instead characterised by a density operator of *mixed states*. This is an important observation. We can now use this to go from a equation that give the time-evolution for the total system to one which only give it for the system of interest. If we where to consider this in the phase space approach to quantum mechanics treated in previous section we could have concluded earlier that this is exactly what is captured in the marginal condition for the Winger function[24]. We can integrate the Wigner function over the environment variables to obtain the reduced Wigner function corresponding to the reduced density operator for our sub-system.

Before proceeding we first mention some word of caution. The separation of a total system into two parts is not always well defined but many situation of physical interest can be model in this way. Moreover, sometimes the affect of the system on the environment is so large that the separation do not serve any use or fails to convey the real physical situation after only a brief period of time (even though at times $t = 0$ it was reasonable). This is however not that common (except in situations which are not of interest to us) and in some sense defeat the entire purpose of the procedure. Often the affect of the system on the environment is smaller that the other way around, and the environment can even be considerer to be unaffected by the smaller system.

3.2 Time Evolution of the Reduced Density Operator: Master Equation Formulation

We will now start the derivation to obtain a equation which describes how our system density operator evolves in time under influence of an environment. For closed quantum

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[24] Recall that the marginal condition is a statement on how to reduce the Wigner function to a sub space of the total phase space. For unrelated degrees of freedom this works in the same way as for x and p, by integrating over the relevant phase space coordinates.

system we know that the density operator satisfy unitary time-evolution, this will not be the case for the reduced density operator. A large part of this is the fact that the trace operation in general is a non-unitary operation. That is, the presence of the environment forces us to consider the trace operation in order to get an expression that describes the dynamic of our system. It is not *a priori* clear that an exact equation for the system time-evolution exist. Indeed, it may not be possible to arrive at such an equation without imposing some sort of approximations.

Throughout this section we will be working in the Schrödinger and interaction picture [10]. A familiarity with the interaction picture is assumed. We begin by first presenting the most general form of the master equation for our case, this consideration serves to establish the nomenclature.

3.2.1 Some Remarks on The General Theory of Master Equations

For simplicity we suppressed the time dependence for ρ_S in Eq.(3.5). If we write it out explicitly we have

$$\rho_S(t) = \mathrm{Tr}_E\left(\rho_{tot}(t)\right) = \mathrm{Tr}_E\left(\hat{U}(t)\rho_{tot}(0)\hat{U}^{\dagger}(t)\right), \tag{3.6}$$

where $\hat{U}(t)$ is the time-evolution operator [10] for the total system and we used the fact that the total density operator evolves in a unitary fashion, i.e. we have $\hat{U}(t) = e^{-i\hat{H}t}$ (for a time-independent Hamiltonian $\hat{H}$). In principle we could use this to obtain the time-evolution for $\rho_S(t)$. This would, however, require that we first determine the time-evolution for $\rho_{tot}(t)$ and then take the trace over the environment. Naturally, following this strategy would not give us anything; we wish to solve the problem by only effectively take the environment degrees of freedom into account. If we instead use the fact that the total density operator satisfy the von-Neumann equation we can take the trace on both sides with respect to the environment variables which yield

$$\frac{d}{dt}\rho_S(t) = -i\mathrm{Tr}_E\left([H(t), \rho_{tot}(t)]\right) \tag{3.7}$$

where $H(t)$ is the Hamiltonian for the total system (here we have no restriction on the Hamiltonian being time-independent). Again this is not an especially useful form for determining the dynamic. The only redeeming factor about Eq.(3.6) and Eq.(3.7) is that they are exact, we have at this time not invoked any approximations. Imposing appropriate conditions [25] (which are consistent with the Markovian approximation, something that we will discuses later) we can write the time-evolution of $\rho_s(t)$ as

$$\rho_S(t) = \hat{V}(t)\rho_S(0) \tag{3.8}$$

which is a nothing but a reformulation of Eq.(3.6) or Eq.(3.7). $\hat{V}(t) = e^{\mathcal{L}t}$ is a *dynamical map* which causes the evolution of $\rho_S(0)$ to the state $\rho_S(t)$. In addition $\mathcal{L}$ is what is known as a *super-operator*: an ordinary operator acts on a function to give a new function, while a super-operator acts on another operator to result in a new operator. As a differential equation we can write Eq.(3.8) in the form

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}\rho_S(t). \tag{3.9}$$

Eq.(3.8) and Eq.(3.9) is the most general form of what is known as *Markovian quantum master equations*. The name "master equation" is used to denote a time-evolution equation for a probability object[25] which is exactly what the density operator is. To proceed we need an explicit expression for $\mathcal{L}$ which is possible to obtain in various ways [25]. We will derive it starting from the formulation of the Hamiltonian for the total system in the next section and then invoke certain approximations.

3.3 Derivation of The Born-Markov Master Equation

We now move on to the task of deriving the Born-Markov master equation (following the method in [25] and [28]). The name comes from two vital approximations made during the derivation.

The Hamiltonian for the total system can be written as (suppressing "hats" for operators to keep the notation clear)

$$H = H_S + H_E + H_{int} = H_0 + H_{int} \tag{3.10}$$

where H_S and H_E are the Hamiltonians associated with the system and environment respectively, H_{int} is the interaction between the system and the environment. In the interaction picture we split up the Hamiltonian into a "free part" H_0 and an interaction part H_{int} to be treated as a perturbation (provided it is sufficiently small). Following the convention of letting operators in the interaction picture be denoted by an explicit time-dependence (if confusion can arise we will indicate the interaction picture by I) we have the von-Neumann equation in the interaction picture

$$\frac{d}{dt}\rho^I(t) = -i\left[H_{int}(t), \rho^I(t)\right]. \tag{3.11}$$

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[25] Recall that the density operator in its fundamental definition contains a factor which says how likely it is that a certain state is populated: $\rho = \sum_i \omega_i \left|\alpha_i\right\rangle \left\langle\alpha_i\right|$ such that $\sum_i \omega_i = 1$.

As characterised by working in the interaction picture the time-evolution of $\rho^I(t)$ only follows from the $\hat{H}_{int}$ part of the Hamiltonian. Integrating Eq.(3.11) we have that

$$\rho^I(t) = \rho(0) - i\int_0^t \left[H_{int}(t'), \rho^I(t')\right] dt', \tag{3.12}$$

where we used the fact that the interaction and Schrödinger picture coincide at times $t = 0$. Inserting this into the original expression, Eq.(3.11), gives

$$\begin{aligned} \frac{d}{dt}\rho^I(t) &= -i\left[H_{int}(t), \left(\rho(0) - i\int_0^t dt' \left[H_{int}(t'), \rho^I(t')\right]\right)\right] \\ &= -i\left[H_{int}(t), \rho(0)\right] - \int_0^t dt' \left[H_{int}(t), \left[H_{int}(t'), \rho^I(t')\right]\right]. \end{aligned} \tag{3.13}$$

Employing the partial trace we get the density operator for the system

$$\frac{d}{dt}\rho_S^I(t) = -i\mathrm{Tr}_E\left[H_{int}(t), \rho(0)\right] - \int_0^t dt' \mathrm{Tr}_E\left[H_{int}(t), \left[H_{int}(t'), \rho^I(t')\right]\right]. \tag{3.14}$$

Assuming that

$$\mathrm{Tr}_E\left[H_{int}(t), \rho(0)\right] = 0, \tag{3.15}$$

which is always possible to satisfy by carefully defining H_0 and H_{int}, this equation reduces to

$$\frac{d}{dt}\rho_S^I(t) = -\int_0^t dt' \mathrm{Tr}_E\left[H_{int}(t), \left[H_{int}(t'), \rho^I(t')\right]\right]. \tag{3.16}$$

This expression is still exact, and to continue we need to impose some approximations. Eq.(3.16) is not an equation that can be easily solved, not even numerically for relatively simple systems. This is because of two features. To start with we have to know the density operator for the total system and its time-dependence. This would mean that we also have to know the time-evolution of the environment which from our system point of view is not of interest. Hence, we like to obtain a evolution-equation that only makes reference to the system density operator. Secondly we have to take into consideration the affect of times $t' < t$ to calculate $\rho_S^I(t)$. If would be desirable to have a equation that only depend on the present time and not on how the system was configuration at all previous times. Hence, we want a time local differential equation in contrast to the existing integro-differential equation. By imposing two approximations we can solve both of these grievances.

Born Approximation: This approximation consist of the assumptions that the coupling between the system and the environment is weak and that the environment is larger in scale than the system[26]. The result of these assumptions is that we can neglect the effect of the system on the environment and thus write the total density operator for all times $0 < t$ as

$$\rho^I(t) \approx \rho_S^I(t) \otimes \rho_E, \tag{3.17}$$

with the equality at $t = 0$

$$\rho^I(t) = \rho_S^I(0) \otimes \rho_E. \tag{3.18}$$

Note that the system density operator is allowed to change drastically as a consequence of the interaction with the environment. Under this approximation, Eq.(3.16), reduces to

$$\frac{d}{dt}\rho_S^I(t) = -\int_0^t dt' \mathrm{Tr}_E \left[H_{int}(t), \left[H_{int}(t'), \rho_S^I(t') \otimes \rho_E\right]\right]. \tag{3.19}$$

We have eliminated the need to know the environments density operator time-dependence, the only knowledge that is required is of its initial state which is a great simplification. To solve the other problem we consider another approximation.

Markov Approximation: The goal of this approximation is to eliminate the need to know $\rho_S^I(t)$ at previous times (i.e we want to get rid of the presence of t' contained in the system density operator in the integral). Before addressing this approximation we write the interaction part of the Hamiltonian in the diagonal product form

$$H_{int}(t) = \sum_\alpha S_\alpha(t) \otimes E_\alpha(t) \tag{3.20}$$

with S_α and E_α some system and environment operators respectively. It can directly be seen that this form can describe any interaction Hamiltonian as a general interaction should be described by products of operators acting on both sub-parts of the total system. If S_α is a hermitian operator then this form have the interpretation that the environment monitor (measure) the observable S_α. This is relevant when one consider measurement induced decoherence. Substituting $H_{int}(t)$ expressed in this form into Eq.(3.19) we have

$$\frac{d}{dt}\rho_S^I(t) = -\int_0^t \sum_{\alpha\beta} dt' \mathrm{Tr}_E \left[S_\alpha(t) \otimes E_\alpha(t), \left[S_\beta(t') \otimes E_\beta(t'), \rho_S^I(t') \otimes \rho_E\right]\right]. \tag{3.21}$$

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[26] In many practical situations it is assumed that the environment is in a thermal state with a given temperature T, and the approximation implies that this state, and thereby the temperature, is unaltered by the coupling to the system.

The partial trace with respect to the environment variables leaves operators which only act in the system space unaffected, and as a result we introduce the *two-time correlator*

$$C_{\alpha\beta}(t,t') = \mathrm{Tr}_E\left[E_\alpha(t)E_\beta(t')\rho_E\right] = \langle E_\alpha(t)E_\beta(t')\rangle_{\rho_E} \tag{3.22}$$

which is the expectation value of the environment operators taken at different times t and t'. Furthermore, if we assume that the environment is in equilibrium (stationary state) we have that the density operator commutes with the Hamiltonian

$$[H_E, \rho_E] = 0. \tag{3.23}$$

As a consequence we can fix the evaluation time of one of the operators in Eq.(3.22) and instead considered the relative time difference

$$C_{\alpha\beta}(t-t') = \mathrm{Tr}_E\left[E_\alpha(t-t')E_\beta(0)\rho_E\right]. \tag{3.24}$$

$C_{\alpha\beta}(t-t')$ is called *the environment self-correlation function* and is a measurement in some sense on how much the environment "remembers" previous measurements. If the environment is large in scale then the disturbance caused by for example a measurement should dispense itself in such a way that the system after a short amount of time returns to the original configuration. Substituting Eq.(3.24) into Eq.(3.21) results in

$$\begin{aligned}\frac{d}{dt}\rho_S^I(t) = -\int_0^t \sum_{\alpha\beta}(C_{\alpha\beta}(t-t')\left[S_\alpha(t)S_\beta(t')\rho_S(t') - S_\beta(t')\rho_S^I(t')S_\alpha(t)\right]& \\ +C_{\alpha\beta}(t'-t)\left[\rho_S^I(t')S_\beta(t')S_\alpha(t) - S_\alpha(t)\rho_S^I(t')S_\beta(t')\right])dt'.&\end{aligned} \tag{3.25}$$

To obtain this expression we exploited the cyclic property of operators when taken under the trace action. Note that the presence of the partial trace now is contained in the environment self-correlation functions. We are now in the position to discuss the Markov approximation.

As previously stated we wish to relax the occurrence of t' in the density operator $\rho_S^I(t')$, contained in the integrand. The key to achieving this lies in how the environment responds to changes caused by interaction with the system. If the environment is sufficiently large and the interaction with the system is not to substantial, any affect on the environment caused by system should in a short amount of time be vanishingly small, if the environment are to be kept at thermal equilibrium. This means that any correlation between different parts of the environment vanish in small amounts of time. More precisely, any characteristic time scales for the environment should be short compared to those of the system. Under the aforementioned assumptions we apply the so called *Markov approximation*. The effect of this approximation manifest itself in a couple of ways. First we note that in Eq.(3.26) the environment self-correlation function $C_{\alpha\beta}(t-t')$ will spike in the value around $t-t'=0$ and be zero when we move away from that time-point. Thus, $\rho_S^I(t')$ will not change during this resetting of the environment. We therefore replace the time argument t' in the density operator by t. Furthermore, we can extend the lower limit of the integral to $-\infty$ as we have $\tau_{Ecorr} \ll t$ which implies $C_{\alpha\beta}(t-t') \to 0$ for $t' \ll t$. With this we can achieve our goal of transforming Eq.(3.26) into a time-local differential equation. Making the change of variables $t' \to \tau = t - t'$ we final have

$$\begin{aligned}\frac{d}{dt}\rho_S^I(t) = -\int_0^\infty \sum_{\alpha\beta} (C_{\alpha\beta}(\tau)\left[S_\alpha(t)S_\beta(t-\tau)\rho_S(t) - S_\beta(t-\tau)\rho_S^I(t)S_\alpha(t)\right] \\ +C_{\alpha\beta}(-\tau)\left[\rho_S^I(t)S_\beta(t-\tau)S_\alpha(t) - S_\alpha(t)\rho_S^I(t)S_\beta(t-\tau)\right])d\tau.\end{aligned} \tag{3.26}$$

What is left to do is to transform this back to the Schrödinger picture. This is not too difficult but somewhat tedious (see for example [28]). The result is

$$\frac{d}{dt}\rho_S(t) = -i\left[H_S, \rho_S(t)\right] - \sum_\alpha \left(\left[S_\alpha, B_\alpha \rho_S(t)\right] + \left[\rho_S(t) C_\alpha, S_\alpha\right]\right), \tag{3.27}$$

with

$$B_\alpha = \int_0^\infty d\tau \sum_\beta C_{\alpha\beta}(\tau) S_\beta(\tau) \tag{3.28}$$

and

$$C_\alpha = \int_0^\infty d\tau \sum_\beta C_{\beta\alpha}(-\tau) S_\beta(-\tau) \tag{3.29}$$

as time-independent objects because the time-dependency is integrated out. Eq (3.27) is *the Born-Markov master equation* which describes the time-evolution for the reduced density operator containing all the physical information about the system. Before we are satisfied one more detail is left to address. By performing these approximations we have introduced the possibility of unphysical solutions that could result in negative density operators [25]. It is however possible to cast the master equation in a form that ensures that the density operator is always positive.

3.4 The Lindbland Form and The Positivity of the Reduced Density Operator

With positivity we mean that the overlap (matrix elements) of the reduced density operator for any time should satisfy

$$\langle\psi| \rho_S(t) |\psi\rangle \geq 0 \tag{3.30}$$

for any pure state $|\psi\rangle$ of the system. Why this condition is important is because of the framework of identifying the matrix elements as probability amplitudes, thus requiring them to be positive.

We will refrain from deriving the general form of the master equation that ensures positivity. Here we will only present the result, the reader is referred to [25] and the original work of Lindblad [29]. To transform Eq.(3.27) into the *Lindblad form* we have to impose another approximation called *the rotating wave approximation.* This consist of assuming that the time-scale τ_E defined earlier is less than the relaxation time-scale of the system τ_R. Note that such a situation is consistent with the assumptions leading to the Markovian approximation. Following this and perfroming some slightly cumbersome calculations (again see [25]) we can write the Born-Marakov master equation in the diagonal Lindblad form

$$\frac{d}{dt}\rho_S(t) = -i\left[H'_S, \rho_S(t)\right] - \frac{1}{2}\sum_\mu \kappa_\mu \left(L^\dagger_\mu L_\mu \rho_S(t) + \rho_S(t) L^\dagger_\mu L_\mu - 2L_\mu \rho_S(t) L^\dagger_\mu\right), \tag{3.31}$$

where the L_μ:s are linear combinations of our original existing operators S_α and goes by the name *Lindblad operators* or sometimes *quantum jump operators*,; and κ effective interaction strength between the system and the environment. The prime over the Hamiltonian indicates that it not necessarily must be the same Hamiltonian as for the isolated system. In other words, the presence of the environment can cause modification to the Hamiltonian describing the system. Such modifications are termed *Lamb shifts* [25].

In the next section we will examine a specific choice of a environment, namely a bosonic bath that can for example describing a electromagnetic field[27].

3.4.1 Example: Environment consisting of Harmonic oscillators

To illustrate the ideas presented above we consider an example which we will only treat in a "glance over" fashion (omitting any detailed calculations). The most common situation is that the environment is thought of as consisting of an infinite set of harmonic

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[27] It is assumed that the reader knows how the electromagnetic field is quantized.

oscillators. This have applications in quantum optics when one examine the quantized electromagnetic field which is exactly described in this way. It is, however, possible to consider a number of different cases, each which is a variant of the harmonic oscillator environment[28]. Apart from determining the particle statistics of the bath (bosons, fermions, spins), one must also specify the specific state. The most common one is, without a doubt, a thermal one, but especially in quantum optical applications it might also be relevant to consider squeezed states. Thus, in principle we have to define which we are dealing with. However, here we will refrain from going into detail on this topic. Instead we will just present some general forms.

With this choice we have the following form of the Hamiltonian for the environment

$$H_E = \sum_k \omega_k b_k^\dagger b_k, \tag{3.32}$$

where the sum over k runs over the different modes. The interaction part of the Hamiltonian can then be assumed to be, in accordance with Eq.(3.20)

$$H_{int} = \sum_j \sum_k \left(g_{jk} b_k + g_{jk}^* b_k^\dagger \right) S_i^\dagger + \left(g_{jk} b_k + g_{jk}^* b_k^\dagger \right)^\dagger S_i, \tag{3.33}$$

with S_i system operators and g_{jk} system-environment coupling coefficients. With the knowledge of the interaction part of the Hamiltonian we can repeat the steps in the derivation outlined above to obtain the Born-Markov master equation for this type of environment, provided that we specify in more detail the initial state of the environment. For more details, see for example [25, 26, 27]. To relate this to the general Lindblad form, it can be seen that the Lindblad operators for a system of a harmonic oscillator one has

$$\begin{aligned} L_1 &= a \\ L_2 &= a^\dagger \end{aligned} \tag{3.34}$$

which represent bosons either leaking/escaping ($\hat{a}$) or entering ($\hat{a}^\dagger$) the system. As expected, for a thermal environment the system reaches a steady state that is also thermal with the temperature determined by the temperature of the bath [27]. A special case is the zero temperature environment with implies that the system ends up in vacuum. Before closing this chapter we will in the next section discuss some aspects of decoherence.

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[28] For bosonic degrees of freedom. Yet, it is possible to formulate the fermionic harmonic oscillator.

3.5 Some Aspects of Decoherence

The topic of quantum decoherence is a large and fascinating subject which touch upon the very foundation of quantum theory. As with almost every subject covered in this thesis we will sadly not have the time to cover it in depth that it deserves. In this section we will only outline some basic facts about decoherence to allow the reader to gain a rough idea of how it is related to open quantum systems. For more information see for example the jovial book [28].

Recall some of the most extraordinary features of quantum mechanics, that in no way can be reconciled with the classical theory, namely the superposition principle and entanglement. These hallmark features of quantum theory can never be observed for particles and other objects in the classical macroscopic world. Still they are present in the microscopic world, as many experiments have confirmed. In order to unify these two diverse results with the classical theory there must be a mechanism that provides a transition from micro- to the macroscopic world with respect to these phenomena. Decoherence is one possible route towards an explanation. Before we continue to talk about decoherence we present a very quick and brief recap on superposition and entanglement to stimulate the readers memory.

Recollect that states in quantum mechanics are represented as vectors in a Hilbert space which is a linear vector space equipped with a scalar product, and thereby a norm. This means that if we have two physical states, describing distinctly different configurations we can form linear combinations of these states which still is a state in our Hilbert space. We write this as

$$|\Psi\rangle = \sum_n c_n |\psi_n\rangle \tag{3.35}$$

with $|\psi_n\rangle$ the "original" states and c_n coefficients. What is remarkable now is that $|\Psi\rangle$ also describes a physical state, a *superposition* of our original distinct states. It is important to stress that this is not a simple statistical expression which tells how likely it is that we have a certain state $|\psi_n\rangle$. In other words this expression for superposition is not a statistical distribution of states which constitute $|\Psi\rangle$. Instead the correct interpretation is that every $|\psi_n\rangle$ is present at the same time in the state $|\Psi\rangle$. Since the quantities $|c_n|^2$ provide the probability to find the system in the corresponding state $|\psi_n\rangle$ (we assume that the different $|\psi_n\rangle$ are orthonormal) it is clear that any phase of c_n is superfluous for determine this probability. Still, the state is not defined solely by the norms $|c_n|$; the phases themselves contain physical information. This is at the heart why quantum mechanics cannot be considered a traditional (classical) probability theory. The presence of the phases of the coefficients make us talk about quantum *coherence* of the physical state. Like in optics, coherent light has a well defined phase.

Assume that we have a total quantum system S that can be thought of as being built up from two subsystems S_1 and S_2. In addition there exist a state $|\Psi\rangle$ describing the total system S. If this state cannot be written as a (tensor) product of state vectors for S_1 and S_2 then we call it *entangled.* In practice this means that if we have a total expression for some state $|\Psi\rangle$ in S composed of states $|\theta\rangle_1$ in S_1 and $|\phi\rangle_2$ in S_2, then we can not separate them in a way that makes in meaningful to speak about the individual states $|\theta\rangle$ and $|\phi\rangle$. In essence, the presence of entanglement prevents the total system S to be divided up into smaller entities which can be examined individually. Or put in other words, all the information about one subsystems is not simply contained in the information accessible by local measurements on that system, full information about that system is only obtained by global measurements on the full system. Hence, this is a cases where the combined system is not simple the sum of its parts. The question then arises, how can we describe a system that is entangled to another one when we only have access to one of them? This is an important question; taking one subsystem to be the environment it is clear that practically we cannot measure the whole environment and still this is what we would typically need to be able to say everything about our system. As we saw above when we introduced the reduced density operators, if we only have access to the system, all information extractable is that contained in the reduced density operator. It is important to note that the trace operation, applied for obtaining the reduced density operator, is not a unitary operations and also not a reversible one. As such, given one reduced density operator for the system there is not one unique state for the system plus environment reproducing this reduced density operator. As mentioned, the reduced density operator is typically not pure but a mixed state. Provided that the full state is pure, a mixed state for the reduced density operator is a necessary and sufficient condition for the two subsystems to be entangled [28].

Turning to how this is related to decoherence we note the following. The presence of an environment acts as a measuring procedure on the system as tentatively mentioned previously. This in turn destroys superposition effects and causes the coherence to be irreversibly lost. This can be attributed to the fact that the environment has recorded what is known as "which-path information", meaning that we can (in principle) make observations of the environment which assure some specific states of the system and thus exclude certain superposition. The information that previously was contained in the superposition considering the system is now carried away into the environment, this can be considered as loss of information in the system to the environment. Hence, the result of interaction for the system with the environment is the loss of superposition and coherence. It is exactly this process which is called *decoherence.* Yet, for the entire system (sub-system+environment) there is no requirement of loss of coherence. It is, however, in realistic situations not possible to measure the entire system in such a way that we can determine how the coherence now express itself. As a final remark, the environment may not only induce decoherence of the system, the coupling can also be of dissipative character meaning that there is an exchange of energy or particles between the system and the environment. In such situations it is not only the information contained in the phases of the coefficients c_n that are lost, but the amplitudes of the coefficients are also affected.

4 Classical and Quantum Chaos

In the last chapter of this part we will shift our focus to the multifaceted subject of chaos. In its essence chaos destroys the greatest goal of the field of physics, the ability to predict future events. The concept of chaos manifest itself in our ordinary lives in a remarkable way, where the most known is the unpredictability of the weather forecast but even at first simple mechanical systems like the double pendulum is doomed to fall into a chaotic motion. What is even more striking in some ways is the fact that this behaviour eluded discovery for so long. For example, both the formulation of general relativity as well as quantum mechanics pre-date the concrete concept of chaos. Why this is unexpected is because that chaos actually is a purely classical concept. Recall that Newton's laws of motion are entirely deterministic. If we thus where to examine a physical situation that allowed itself to be modelled as a Newtonian system we would expect that with sufficient information we could determine its dynamic for all future times. However, for a great many situations this is not the case. Moreover, this is not a shortcoming of the Newtonian formulation but something that seems to be inherent in nature itself. It is the goal of this chapter to give a small overview of this strange and fascinating subject.

With the description of chaos as a classical phenomena one is left to wonder how this fits together with quantum mechanics. If the classical macroscopic world can exhibit chaos then should not also quantum mechanic show some signs of chaotic behaviour? After all, we usually treat quantum mechanics as the more fundamental theory that can both describe the microscopic world as well as the macroscopic world in the classical limit. Yet, quantum mechanics lacks the usual properties and structures that we associate with chaos. If chaos exists in the quantum world then its occurrence are shrouded in mystery compared to what we classically would expect. This seems to be another aspect of the fundamental "strangness" of the quantum theory. Even more, some regard this, together with the combination of general relativity and quantum field theory, as the largest remaining obstacles related to the fundamental formulation of quantum theory [30]. The researched field of quantum chaos is as a result still a active one with new developments regularly. However, it is important to remember that as of now there does not exist any agreed upon unified definition of what quantum chaos is.

The outline of this chapter is as follows. We start with some quick remarks about integrability in the classical theory, this serves to set the stage for a brief discussion on the KAM-theorem, ergodicity and finally chaos. The backdrop for these subject is the classical theory. It is important to establish these concepts in a setting that is familiar to promote understanding when we later try to borrow these concepts into quantum mechanics. In some sense this is even more imperative when our choice of quantum formulation is the phase space formulation from chapter 2. After the discussion on classical chaos theory we shift our focus to quantum chaos. We will first discuss the important fact that chaos can not be lifted over in any apparent way into quantum mechanics due to how the theory is fundamentally formulated. After that we discuss some of the common methods of trying to charactering chaotic occurrence in the quantum world.

Before proceeding we have to make a comment about the scope of the present text. The topic of chaos have grown to a subject that is so large that not even any single book wholly dedicated to this area can be expected to cover everything. This is even more true for a short thesis. We will omit a large amount of theory, both in the classical part as well as in the quantum part. The present text can at most be considered a brief introductory summation. For a more thorough treatment see for example [25-31].

4.1 Remarks on Integrability in the Classical Theory

The quest to examine a classical system starts by postulating some dynamical property contained in an expression for the force, Hamiltonian or Lagrangian. After this crucial first step comes the often overwhelm task of trying to obtain the equations of motion for this system. Having obtained the equations of motion the question comes to solve them, whether it can be done analytically or numerically. Is there any systematic way to determine if a system can be solved in such a way what the result can be formulated as a closed analytical answer? This question constitute the investigation of the *integrability* of the considered system [31]. Moreover, the presence of integrability in a system seems to imply regular motion in phase space which exclude any chaotic tendency [31].

Consider a system with N degrees of freedom (number of particles as well as number of position q_i directions). The phase space that we use to describe this system consists of $2N$ dimensions (to every position direction we have a corresponding canonical momenta p_i). We call this system *integrable* [36] if it exists S constant of the motions that are mutually independent of each other:

$$I_i(p_1, ..., p_n; q_1, ..., q_N) = C_i \tag{4.1}$$

for $i = 1, ..., N$ such as that $S \leq S$. In other word, an integrable system has an equal or larger number of constants of motion than degrees of freedom. The constants of the motion must in addition satisfy the condition

$$\{I_i, I_j\} = 0 \tag{4.2}$$

this vanishing of the Poisson bracket between I_i and I_j is known as *involution.* The existence of constants of the motion restricts the flow in phase space to a lower dimensional subspace. Furthermore, it allows for the construction of action-angle-variables (see [16]). In these variables the flow for an integrable system is confined to a $(2N - S)$ dimensional torus in our original $2N$ phase space.

It turns out that uncovering whatever a system is integrable or not can be quite difficult. The constants of the motion can be determined from the celebrated *Noether's theorem* [38], at least in principle. For space-time symmetries this is usually not to hard (energy, momentum and angular momentum). These are, however, not the only symmetries that can exist. In addition we can have what is called "hidden" symmetries [36] which are much more difficult to identify. In the end we are often in the position where we can not in any practical sense identify what or if there are constants of the motion.

4.1.1 The KAM-Theorem

Assume that we know a Hamiltonian H_0 which is integrable. We know ask ourself what happens if we add a small symmetry breaking perturbation to this

$$H = H_0 + \epsilon H_{pert} \tag{4.3}$$

where ϵ is a "small" parameter regulating the strength of the perturbation. Does this addition of a small perturbation render the new Hamiltonian non-integrable and thus destroying all characteristics of a integrable system? In the last section we stated that the motion in phase space for an integrable system is confined to an N dimension torus meaning that we can formulate this question as an inquiry if the invariant torus survives under small perturbations. The answer to this question is provided by what is known as the *Kolmogorov-Arnold-Moser theorem* (KAM-theorem) [16, 37] which asserts the following: *If an original integrable Hamiltonian H_0 is perturbed by the addition of a new term ϵH_{pert} which makes the total Hamiltonian H non-integrable then the motion in phase space is still confined to a N dimension torus, provided that the perturbation is small*[29]. The proof of this theorem is notoriously known to be cumbersome, see [31, 36, 37] for an outline to the proof. The strength of the KAM-theorem is the assertion that there exist stable solutions to the equations of motion stemming from a non-integrable Hamiltonian in the case of small perturbations. By allowing the

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[29] A second, often stated, condition on resonance (frequencies) is also necessary in principle. This condition comes from the construction of action-angle-varaibles and the perturbation theory used to prove the theorem. In addition a number of other criteria is also needed for the proof (see the references for the outline of the proof above).

perturbation to grow we can explore the transition from regular behaviour to what with large perturbations becomes, chaotic behaviour.

4.1.2 Ergodicity

To explain the concept of ergodicity we must in general resort to action-angle-variables explicitly, something that we will avoid in this thesis. Instead we will give a qualitative explanation.

If we again turn to an integrable system and the resulting invariant torus we can note that a periodic motion will be restricted to certain part of this torus (as it is forced to return to its starting value after each period). For quasi-periodic motion we have that after one period the system returns *almost* to the starting position but not quite. After some time this means that the system will gradually explore the whole available phase space as it always misses to return to its starting value. We can express this more concretely by computing the time average of some quantity

$$\langle B \rangle_t = \frac{1}{T} \int_0^T B(x(t))dt \tag{4.4}$$

if this is equal to the phase space average for the same quantity (taken with respect to a phase space distribution function $p(x)$)

$$\langle B \rangle_p = \int B(x)p(x)dx \tag{4.5}$$

then we say that the system is *ergodic* [32]. To ensure this behaviour it is often common to take the limit $T \to \infty$ as to allow the system to truly spread out in phase space. From the explanation above we can see that a quasi-periodic system is ergodic. The concept of ergodicity is of central importance in statistical mechanics and constitute its own mathematical field. We are interested in it because of its ability to hint at chaotic behaviour. From the KAM-theorem we know that as the perturbation grows the torus deforms and gradually breaks up, and in the process the phase space flow spreads out over all of phase space (the behaviour transforms from quasi-periodic to aperiodic). With that said we have to stress the fact that a chaotic system is ergodic but all ergodic system are not chaotic (as is obvious from the consideration of integrable systems that possess quasi-periodic dynamic). Furthermore, ergodicity is related to what is known as *mixing* which some take as a defining property of chaotic dynamic [37].

4.2 Classical Chaos

The road to “classical” chaos is still one which is debated (although not nearly as much as that of quantum chaos). Usually a system go from regular to chaotic evolution when certain parameters are varied in for example the Hamiltonian. Why, however, chaos occurs for specific values of parameters are not in general always known. Moreover, we have that many characteristic aspects of chaos can present themselves in non-chaotic systems, as was mentioned with ergodicity previously. With this said, there are at large consensus on what chaotic behaviours should imply.

The task of determining if a system is chaotic is often problematic. To start with we have to septate what is known as “local” chaos to that of “global” [30]. It is possible that some sub-part of our system for example shows sensitivity to initial conditions while other parts do not. The problem of identifying global chaos is still not entirely understood. For practical purpose we will focus on "local" chaos.

4.2.1 Criteria for Chaos

For an system which is non-linear[31] and non-integrable we have the following criteria that a dynamical system should fulfill in order for us to identify the presence of *chaos* [34].

- “Aperiodic long-term-behaviour” which means that there are trajectories in phase space that are not periodic or quasi-periodic as we let the time period go to infinity.
- “Deterministic” implying that the system is not affected by noise or other random effects. The tendency of chaos is something that is inherent in the non-linear nature of the system and not caused by random influences.
- “Sensitive dependence of initial conditions” meaning that trajectories in phase space which start closely together separate exponentially fast as time progress. This is described by a positive *Lyapunov exponent*. We will talk a bit more about these exponents later.

In addition to these conditions some authors also use the following criteria (among a number of others), which we state for completeness.

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[30] This is however not a distinction we will devote any large amount of time on.

[31] Not all non-linear system have to be chaotic, but all system that exhibits chaos are necessary non-linear.

- "Positive *Kolmogorov-Sinai entropy* (KS entropy)". This entropy is related to deformation of sets in phase space under some time-evolution. Related to this is the concept of mixing and ergodicity. Yet, the KS entropy can be expressed as a function of Lyapunov exponents and thus we will not devote any more time to this topic.

For sources containing more methods for identifying chaos see [35, 36, 37]. In practice, these conditions are often hard to identify as stated before. Consider for example the second point. It is in many situations almost impossible to rule out any form of noise, even in the most controlled lab environment. Still this condition is a necessity to separate the behaviour of chaos from other complex behaviour caused by random effects which is explained by a different theoretical framework.

In the three first points the only quantity that is undefined is the Lyapunov exponent which we will now explore in little more detail. If we examine a given point in phase space where a trajectory starts we can ask ourself what happens if we change the starting point by a small amount δ. Using (for example) linear stability analysis [34, 39] we can construct a measurement on how much the unmodified and modified starting point affect the corresponding trajectories. The separation between the two trajectories fulfils

$$\delta(t) \sim \delta_0 e^{\lambda t} \tag{4.6}$$

where the zero indicate the starting separation and λ is the *Lyapunov exponent*. For negative λ we have the usual behaviour that we would expect. A small change in the initial starting point dies out as time progress. However, for a positive λ we have the direct opposite. Even the smallest change will quickly cause the separation between the two trajectories to increase, rendering two completely different processes. This is what we mean with "sensitive dependence of initial conditions". Eq.(4.6) is valid for each dimension in phase space, thus we have many different Lyapunov exponents, one for each direction in phase space. For a Hamiltonian system the sum of all the Lyapunov exponents have to equal 0 to preserve the flow (Liouville's theorem). It is sufficient if only one of the Lyapunov exponents is positive for chaos to set in.

4.2.2 Tools For Analysing Chaotic Behaviour

The examination of chaotic dynamic is often a complicated topic. Most of this comes from the non-linear and non-integrable character, but also from the fact that chaotic behaviour only happens in higher dimension (Hamiltonian) systems where the number of dimensions of phase space is at least three. To aid us in our struggle there exist a number of tools that can be of help to the analysis. We will not have the space to cover the tools in any depth, for more detail see the specialised literature [33, 34]. Here we will only present the perhaps most famous example, namely the *Poincaré map* [16, 39] (also known as the Poincaré cut or surface of section).

The idea behind this procedure is to utilise subspaces of the considered phase space. Concretely we construct a surface that is perpendicular (the cross section) to the flow direction. This surface will have $N-1$ dimension. Each time the flow (classical trajectory) intersects this surface we mark the corresponding point. After some period of time we will be able to see a pattern (for regular systems) or the lack thereof (irregular systems). Often we have that the energy of the system is a constant of the motion, resulting in the reduction of our effective phase space to $N-1$ dimensions. Then the Poincaré cut can further reduce the number of dimensions by one to ease the visualisation. In addition, we also have the advantage that our original continuous phase space is transformed to a discrete one represented only by points, which in some instances is practical. It is possible to use the Poincaré map to examine the stability of trajectories and get an idea of the possiblity of chaos in the system (although it is problematic to unequivocal determine if the system is chaotic from this map in higher dimensions). In figure (1) a Poincaré map is shown in three dimensions.

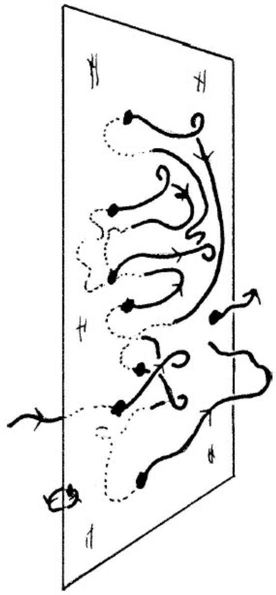

Figure 1: An example of a Poincaré map in three dimensions. Note the periodic curve in the lower left corner and the resulting difference in the map compared to a non periodic trajectory. Figure is taken from [40].

4.3 Quantum Chaos

Having quickly summarised the theory of classical chaos we instead turn to quantum manifestations of chaos. The concept of "quantum chaos" is still to this day somewhat controversial and some authors avoid the name altogether. The reason for this controversial are the fundamental differences between the classical theory and the quantum one which prevent the definition of chaos from section 4.2.1 to be applicable on quantum mechanics. In the next section we will illuminate some of these difficulties. What is interesting to note is that the problem of defining quantum chaos is also present in classical wave-system which we know share many properties with quantum mechanics. Thus, instead of quantum chaos some speaks about "wave-chaos". We will adhere to the first name to emphasise that we seek a description or analogy of chaos valid in the microscopic realm.

With these problems, why do we still insist on examining and talking about the concept of quantum chaos? In the introducing section to this chapter we mentioned that we consider quantum mechanics the more fundamental theory which in principle should be able to explain both the microscopic as well as the macroscopic world. In contras, we know from experience that classical mechanics is only valid in the macroscopic world. There should, however, exist an intermediate length scale (mesoscopic) where the predictions of classical mechanics are "sufficiently" valid. At the same time we could also use quantum mechanics at this scale. The result would be that we have two models of the same system. If now the classical description exhibits chaos then in order for us to reconcile these two descriptions we expect the quantum formulation to also exhibit some behaviour related to this chaotic tendency which is present in the classical description. We suspect that the occurrence of chaos expresses itself differently in the two theoretical frameworks, but in the end is caused by common factors.

4.3.1 The Problem of Defining Chaos In Quantum Mechanics

Before addressing the topic of this section we will first try to transfer the concept of integrability to quantum mechanics. The resulting definition will contain fatal flaws [41]. The question of integrability in quantum mechanics is not as straightforward as in classical mechanics. Nevertheless, we proceed and state the most common definition. Considering a quantum system consisting of N degrees of freedom we say this system is *integrable* [36] if there exist N operators (which is defined globally) $\hat{I}_m$ for $m = 1, ..., N$, for which their mutual commentator vanish:

$$\left[\hat{I}_m, \hat{I}_n\right] = 0 \tag{4.7}$$

for every combination n and m. The implication of this relation is that we can construct common eigenstates for the operators $\hat{I}_m$ and $\hat{I}_n$. In addition, if we denote the i:th eigenvalue to the operator $\hat{I}_m$ as $e_m(i)$ we can construct a one-dimensional subspace to the given Hilbert space by collecting the set of eigenvalues $\{e_1(i), e_2(j), ..., e_N(k)\}$ for the N operators stated above. This collection of eigenvalues are called *good quantum numbers* and are related to the classical concept of constants of the motion. We also note that we can state the concept of integrability in the phase space formulation of quantum mechanics by using the Moyal bracket from chapter 2 instead of the commutator. The advantage of this is that the connection to classical integrability is more evident[32]. With this we can seemingly extend the definition of integrability to quantum mechanics. Important to stress is that this definition is inadequate from a strict point of view. It does serve to illustrate the concept. Furthermore, this is the first indication that quantum chaos is a hard topic to define.

In accordance with the definition of chaos given in section 4.2.1 we now try to extend the definition to a quantum system. A quantum system is characterised by a wave-function $\psi(\{x\}, t)$[33] and by its time-evolution which is given by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(\{x\}, t) = \hat{H} \psi(\{x\}, t) \tag{4.8}$$

with the Hamiltonian H which in many cases can be taken to be on the form $H = \frac{\hat{P}^2}{2m} + V(\{\hat{x}\})$. We have encountered our first problem in defining chaos in quantum mechanics. The Schrödinger equation is a linear-partial differential equation. Thus, we lack the non-linearity which we associate with chaos. We may wonder if the given form of the Hamiltonian is to blame for this linearity, but if we want to preserve the characteristic properties of quantum mechanics, like the superposition principle, then the Hamiltonian must linear. This is the most well known problem among the layman. It is, however, only one among many problems which we will encounter trying to extend our definition of chaos into the quantum world.

Examining the most popular criteria for chaos, the sensitivity to different initial conditions, we will see that also this will falter. The first reason for this is that we cannot speak about points in quantum mechanical phase space. Heisenberg's uncertainty principle prohibits us from knowing the exact momentum and position, thus

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[32] By imposing that this classical limit be well defined the problem of integrability in quantum mechanics can be solved, with one important caveat. Not all relevant operators have a well defined classical limit. Hence, this method of solving the problem with quantum integrability can not be universally valid.

[33] Or a state $|\psi(t)\rangle$. Here we choose the representation of the state in position space, hence the wave-function $\psi(\{x\}, t)$.

preventing the specification of the system to one point in phase space. Moreover, we saw in chapter 2 that the classical correspondence to a quantum state, which we represent in phase space by the Wigner function, is a Liouville probability distribution. This is certainty not the same as a point. In fact, the topic of defining chaos in statistical mechanics with attached Liouville probability distribution is no trivial matter! This is largely a consequence of Liouvilles theorem and that it is possible to create the Hilbert space consisting of Liouville probability distributions [42], meaning that many of the problems of defining chaos in quantum mechanics where already present in the classical branch of statistical mechanics! Yet, there are even more problems in the quantum world. One of the ways in which we can understand chaos in statistical mechanics is by what is known as *stretching and folding*. In the presence of Hamiltonian (i.e. conservative energy evolution) chaos, a Liouville probability distribution will expand in a certain direction where the Lyapunov exponent is the largest, at the same time it must conserve the total volume meaning that it has to shrink in another direction. After some time it will hit the boundary of the allowed phase space, it then "folds" over [39]. This process can continue indefinitely until the original distribution possess an infinite amount of substructure details, in other words a fractal pattern (this is only one among many of the connections between fractals and chaos). For the Wigner function we can however not have this process of stretching and folding as it lacks the possibility to exhibit structure on scales less than $\hbar$ (see chapter 2), in this sense the Wigner function is much smoother than its classical counterpart[34] [44]. If were, however, to disregard this issue and instead postulated that the overlap between quantum states is the quantum mechanical analogue to distance between trajectories we would have for two states, where one is slightly perturbed compared to the other

$$\langle\psi(x+\delta x,t)|\psi(x,t)\rangle = \langle\psi(x+\delta x,0)|\,\hat{U}^\dagger\hat{U}\,|\psi(x,0)\rangle = \langle\psi(x+\delta x,0)|\psi(x,0)\rangle\,, \quad (4.9)$$

where we used the fact that the time-evolution is given by the unitary time-evolution operator $\hat{U}$, and as a consequence $\hat{U}^\dagger\hat{U} = \hat{1}$. Thus, we find that the overlap for two states is constant in time. In quantum mechanic there exist no exponential sensitivity to perturbation in the states. Hence, we see that this definition of chaos is inapplicable to the quantum theory.

Turning our attention to the first condition in section 4.2.1 it can be proven that for a general quantum system with discrete energy spectrum we have what is known as

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[34] This is actually true with some modifications. The Wigner function can show fine structure in its interference pattern [43]. Still, the Wigner function does not exhibits stretching and folding in the same way as a classical distribution do (this is related to the property mixing mention before and the fact that the Wigner function cannot exhibit this feature [44]).

the *Quantum Recurrence Theorem* [30, 45]. This theorem state that during the time-evolution of a given wave-function it will infinitely many times return arbitrary close to its starting configuration. This behaviour does not necessarily have to be the same as periodicity (the time scale must not be the same for this recurrence) but it is at least quasi-periodic. The result is that we seem to always have at least quasi-periodicity in our quantum systems which is something that excludes chaotic behaviour in the classical sense.

In the end we only have one surviving condition left from section 4.2.1 and that is the second point. Even with its statistical properties, quantum mechanics is a deterministic theory. With sufficient initial conditions and boundary conditions we could in principle predict all future behaviour (again within the confinement of the statistical interpretation of quantum theory).

After this section all hope of charactering quantum chaos may seemed lost. Yet, there is still hope. In the next section we will explore outlets for chaos in quantum theory, given that we *know* that chaos exist in the corresponding classical system.

4.3.2 Outline To Methods of Characterising Quantum Chaos

Even though we cannot talk about chaos in a traditional sense in quantum mechanics, it is found that quantum systems with their classical counterparts being chaotic show qualitatively different behaviours than those with regular classical counterparts. In the most strict way we can *only* speak about quantum chaos when we can relate our quantum system to a classical one where chaos is present. Not all researchers are in agreement when it comes to this as there exist methods that does not explicitly require this connection. Although this may be the case none of these methods are consistent in the way that they work in every situation [3, 32]. There still exist systems where experimental results differs from what theory predicts. For the models where no explicit reference to the classical theory is made this shortcoming is more severe because it illustrates some flaw within the theoretical reasoning.

In addition we have in the quantum world, problem in distinguish semi-regular behaviour from that of total irregular behaviour. In classical systems we encounter situations when the dynamics is mixed, meaning that parts of phase space displays regular evolution while other show fully chaotic motion. This is best illustrated by the KAM-theorem. When we want to compare a given quantum model to the corresponding classical one, it is helpful if we can ensure that the classical system exhibits full chaos, otherwise we can happen on the cases where no apparent effect of chaos manifest itself in quantum behaviour because we are in a area where classically there is no irregular tendencies. Thus, to ease the establishment of connections between classical and quantum chaos we only examine systems with fully developed chaotic behaviour. Even with this distinction there will in practice often be areas where the behaviour is approximately regular, at least on small time scales.

There exist three main methods of characteristic quantum chaos that is in popular use at the moment [3, 37]. Each one of these have strength and weaknesses depending on the situation. Moreover, connections between the different methods have in some situations been established.

1. **Semi-Classical Methods:** This procedure combines the path integral formulation of quantum mechanics with classical, or more accurate semi-classical, approximations. Many of these results surprisingly stem from the failure of the "old" quantum theory to quantize non-integrable system. It was Gutzwiller [35] who realised how the old quantum theory could be modified and combined with the rigours path integral formulation to yield an approximate method for non-integrable quantum systems. This approximation can be considered a generalisation of the WKB-method which is only valid for a integrable system. The method illustrates the interesting occurrence of classical "scars" in quantum mechanical spectra which depend on the regularity of the corresponding classical system. To limit this thesis to a reasonable length, we will not focus on this method any further, the interested reader are referred to [33, 35, 37].

2. **Perturbation of The Hamiltonian:** We can mimic the sensitivity to initial conditions by instead considering perturbation to the Hamiltonian describing the dynamic of the system
   $$\hat{H} = \hat{H}_0(\lambda) + \hat{V}(\delta\lambda) \tag{4.10}$$
   in such a way that we let one state evolve according to the original Hamiltonian $\hat{H}_0$ and the other according to $\hat{H}$. If we then calculate the overlap squared we have
   $$|\langle\psi(0)|\,\hat{U}^\dagger\hat{U}_0\,|\psi(0)\rangle|^2 = |\langle\psi(t:\lambda)|\psi(t:\lambda+\delta\lambda)\rangle|^2 = F(t,\delta\lambda), \tag{4.11}$$
   where $\hat{U} = e^{-i\hat{H}t/\hbar}$ and $\hat{U}_0 = e^{-i\hat{H}_0 t/\hbar}$, and where we introduced the *fidelity* $F(t,\delta\lambda)$ in the last line. It can be shown that this measurement can exhibit exponential sensitivity on the perturbation $\delta\lambda$ [44, 46]. Although it may seem that this method does not rely on the occurrence of a classical counterpart system in order to verify its validity one should consider systems with a well defined classical counterpart [3]. For states who's classical counterpart lie in a chaotic domain we get the descried result, sensitivity to initial conditions. For those that do not, the fidelity does not show this behaviour [46].

3. **Random Matrix Theory:** Of these three methods, perhaps the most interesting is the one which utilises the theory of random matrices [3]. We will dive into this subject in a bit more detail in the next section. Briefly, we can say that in random matrix theory we abandoned our desire to specify the Hamiltonian in any detail. The reason for this is often that the system under consideration is far to complex to capture in any reasonable way. A consequence of this is that the spectrum will fluctuate in a certain way. By distinguishing between different distribution functions describing these fluctuations we can say something about the underlying dynamics. Note that this method can work in principle without any direct connection to a classical system, although the physical analogue to a classical system is helpful to understand the spectrum.

In the reminder of this chapter we will deal with random matrix theory and *quantum thermalization*.

4.3.3 Random Matrix Theory

As customary in this thesis, we will make no claim of covering this subject in its wholeness. With that said, this section can hopefully be thought upon as a short introduction to an interesting topic. For more information see for example [3] or the more mathematical literature [48]. The theory of random matrices have applications in many diverse branches in physics.

In section 4.2.1 we discussed the problems one encounters when trying to define chaos in quantum mechanics. We even saw that it is problematic to define quantum integrability in a straightforward manner in quantum mechanics. Even then we did present a method which mimics the classical form. If chaos where to occur in the quantum world we suspect that it will follow our classical reasoning and take place in non-integrable systems regardless of how quantum integrability is defined strictly (non-integrability is expected to be the rule rather the exception). What these systems usually have in common is that they in some sense can be considered "complex" or complicated. The dynamical properties are often coupled between parts of the system leading to an inability to solve the system in any simple way. Furthermore, constants of the motion for the system are few or non existing. Prime candidates for such complicated systems can for example be highly exited atoms, nucleus consisting of many components, or many-body systems in general. In additions to the failure of our classical definition of chaos we also have to be careful what we treat as "good" observables in the quantum theory. For example, it is not practical to try and measure the position or momentum of particles, like atoms. In practice, what is typically measured is the energy spectrum. This spectrum is the associated energy-eigenvalues to the Hamiltonian describing the system. Moreover, these eigenvalues determine the evolution of the system by the spectral theorem [37]. We suspect that by examining the spectrum of a system we can determine whether the underlying dynamics is integrable or non-integrable as the distribution of eigenvalues behaves in a different way for the two cases. If by comparing with corresponding classical models we can detect a difference in how the eigenvalues are distributed we can take this as an indication of quantum chaos. Yet, this method does not rest on any connection to classical models and can thus be applied to purely quantum mechanical systems.

Before considering the more interesting case of non-integrable systems we first examine the unlikely scenario where a complicated system is integrable[35]. From the defining condition of integrability we know that this system possesses constants of the motion equal to the number of degrees of freedom. Each constant is related to a corresponding operator that commutes with the Hamiltonian. It is this property that results in *degeneracies* [10]; several (or pair) different states of the system share the same energy-eigenvalue. For a complicated system we will have a large number of degrees of freedom and necessarily many degenerate energy levels. Even though the system could in principle be solved (as it is integrable) we have no guarantee that this can be done by reasonable amount of work[36]. What is even worse is that this solutions will be very specific to just this system, often to certain parameters that preserve the needed symmetries. Even the slightest change will render our previous solution invalid and requiring reconsideration to obtain a new solution. Instead of all this we will try to make some general predictions of systems that are integrable from the fact that they possesses many degenerate energy levels. Besides the degeneracy we also assume that the different degrees of freedom are isolated from influences between each other (as would be the case in classical mechanics). The result is that for a highly exited system we suspect that the energy-eigenvalues are distributed in a random fashion.

Consider the difference between two energy-eigenvalues $s = e_{i+1} - e_i$ (energy *spacing*), organised in such a way that $e_{i+1} > e_i$. If e_{i+1} and e_i are random then so to is the spacing. This spacing will in turn be different for each neighbouring pair of eigenvalues. We want to obtain a distribution $P(s)$ describing the different possible values of the spacing. This is done by first define a function $f(s)ds$ that is the probability to find an energy-level in the interval $e + s \rightarrow e + s + ds$ from a given level located at e,that is

$$f(s)ds = \frac{1}{D}ds, \tag{4.12}$$

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[35] Integrable systems are typically found in lower dimensions, i.e. in one dimensional systems.

[36] The solutions may, for example, be given by complex integral equations as is typical in *Bethe solutions*.

where D is the assumed average spacing. The probability that there is no energy-level in an interval $e \to e+s$ can be expressed

$$\int_s^\infty P(s')ds'. \tag{4.13}$$

To form our total expression for $P(s)$ we note that the assumption that the energy-eigenvalues are uncorrelated allows us to write the probability of finding a spacing scale within the interval between s and $s+ds$ as

$$P(s) = f(s)\int_s^\infty P(s')ds' = \frac{1}{D}\int_s^\infty P(s')ds. \tag{4.14}$$

Taking the derivative of both sides with respect to s results in

$$\frac{dP}{ds} = -\frac{1}{D}P(s) \tag{4.15}$$

which is trivial to solve, the result being

$$P(s) = \frac{1}{D}e^{-\frac{s}{D}}. \tag{4.16}$$

This is the well known *Poission distribution* which here describes the probable amount of spacing between two energy-levels. In figure (2) we can see a plot of the Poission distribution (along with a hint to a future result). What is noteworthy is that the most likely spacing between two consecutive energy-levels is zero, that is to say they are identical. This is a result of the degeneracy related to the underlying integrability of the system. The present of a Poission distribution for the energy spacing can be taken as an indication for regular dynamical behaviour underlying the system.

Is it possible to get a corresponding distribution for the spacing when the underlying dynamic is non-integrable? In that case we suspect that the degrees of freedom are coupled to each other and the resulting energy-eigenvalues are repelled.

Consider a complicated non-integrable system. This system cannot be solved analytically, the only options is to attempt numerical approaches or invoke appropriate approximations. This however rest on fact that the Hamiltonian is specified in detail (precise number of particles, which exited state each is in etc.). This fact will be highly sensitive to the precise state of the system (small difference in the configuration can have an unexpected effect on the dynamics as is the case in classical chaotic systems). Yet, for a complicated system, can we always formulate the Hamiltonian in such a way that it captures in detail fully the dynamics of the system? A reasonable answer would be no, there is always some interaction or factor which eludes us. Moreover, even if the

Hamiltonian is stated it will be highly specific to this configuration. Results obtained by utilising method to solve this case would then not be valid for a system that is just slightly changed compared to the original. Furthermore, in the cases where the interaction between different parts of the system is strong even the often used method of perturbation theory can be invalid. The perturbation simply overpowers the "free" part of the Hamiltonian. The result is that we are in a position where we cannot state a Hamiltonian in a such a way that we with certainty can say that is exactly faithful to the current configuration, or use perturbation theory to any success. But what if we embrace our inability to know the Hamiltonian with certainty in any exact form? If our system is complex then it should consist of many particles and interactions, and the details remain unknown. Comparing many different systems, the detail structure of particles and interactions will vary. In the end, the Hamiltonian will appear to be almost *random*. Thus, we can expect a nearly universal behaviour for the spectra corresponding to these complex systems resulting from random Hamiltonians. An important distinction is in place. The elements of the Hamiltonian are allowed to be random, as long as the Hamiltonian satisfy some symmetries which will be discussed below. These symmetries are the only information about the system that enters into the analysis which is quite remarkable.

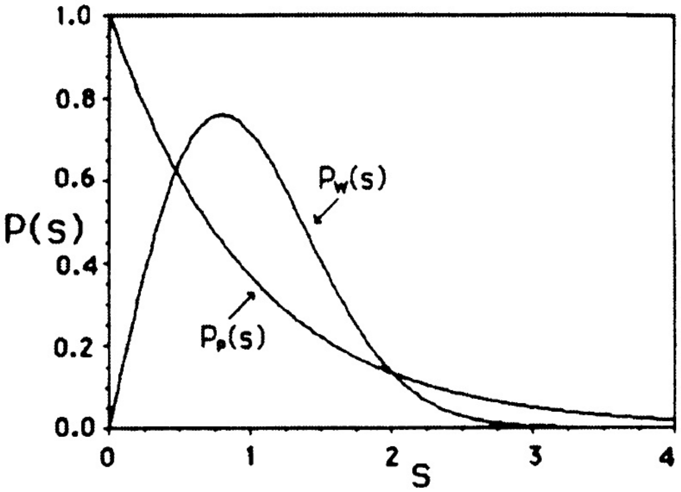

Figure 2: A illustration of two different distributions describing the level spacing s. $P_p(s)$ is the Poission distribution (here $D = 1$), while $P_w(s)$ is the Wigner surmise (also for $D = 1$). Note especially the radical difference for $s \approx 0$. Figure is taken from [36].

To summarise we consider matrices (Hamiltonians in a matrix representation) where we minimise the amount of information accessible with the only exception being relevant symmetries. From this we construct a statistical ensemble of matrices which satisfy the following two conditions [37] (this is the origin of the name *random matrix theory*)

- The matrix elements are statistical independent of each other. This means that each element in the Hamiltonian matrix is an independent random number. The implication of this is that the distribution of a whole matrix can be factorised into a form consisting of its independent, individual probability parts

  $$P\left(H = \{H_{i,j}\}_{i,j}\right) = \prod_{i,j} p_{i,j}(H_{i,j}) \tag{4.17}$$

  where $H_{i,j}$ is a matrix element in the Hamiltonian and $p_{i,j}(H_{i,j})$ is the probability for the i, j element in the Hamiltonian.

- The choice of basis when one represents the Hamiltonian in matrix form should not influence its statistical properties. For this condition to hold the results must be invariant under basis transformations. It is this property that is affected by what symmetries the matrix possesses.

The first condition is necessary in order to minimise the amount of information in the Hamiltonian and is of great help when deriving the distribution resulting from a random matrix. The second condition results in three different cases, depending of present symmetries. But which symmetries are important for this condition? Recall that continuous (infinitesimal) symmetries are characterised by generators [10, 47]. These symmetries reduce the number of non-zero elements in the Hamiltonian by enabling us to write it in block diagonal form. Hence, they only reduce the number of elements in the Hamiltonian but make no restriction on how the matrix blocks must behave under transformation. It is instead the discrete symmetries that impose restrictions on the form of the Hamiltonian matrix. Most important is the time-reversal symmetry. Depending on if we can expect real, both real and complex, or quaternion[37] elements in the Hamiltonian we get three cases for how a transformation must be performed to fulfil the second condition. For more information about symmetries and how they play into the theory of random matrices see [3, 36]. To illustrate the

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[37] Quaternion numbers can be viewed as a extension of the complex number system into four-dimensions (where the complex numbers extend the real numbers to two-dimensions). The use of these numbers are caused by consideration of spin $\frac{1}{2}$ systems which are not rotationally invariant [36].

theory we will consider one of these cases, even though some of the results are general in the sense that slightly modified forms are true for the other two cases. In addition, we will restrict our attention to a 2 x 2 matrix, the result for N x N matrices is more complicated [3]. With that said the result for a 2 x 2 matrix is a surprisingly good approximation to the general case.

Our starting point is the symmetric real Hamiltonian matrix with the three elements H_{11}, H_{22} and H_{12}

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{12} & H_{22} \end{bmatrix}.$$

We know from the first condition that we can state the probability for the entire matrix as a product of the elements

$$P(H) = p_{11}(H_{11})p_{22}(H_{22})p_{12}(H_{12}). \tag{4.18}$$

Furthermore the second condition also has to be satisfied. For a symmetric real Hamiltonian the condition is that it has to be invariant under orthogonal transformations [49]

$$P(H) = P(OHO^t) = P(H'). \tag{4.19}$$

Lastly we also have our familiar normalisation condition on the distribution

$$\int dH_{11}dH_{22}dH_{12}P(H) = 1. \tag{4.20}$$

The matrix representation of an orthogonal transformation is well known in two dimensions and can be expressed as a rotation around an angle θ [16]

$$O(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}.$$

In the limit $\theta \to 0$ (infinitesimal) we have the form

$$O(\theta) = \begin{bmatrix} 1 & -\theta \\ \theta & 1 \end{bmatrix}.$$

The transformed Hamiltonian elements then become in this limit

$$H'_{11} = H_{11} - 2\theta H_{12}, \tag{4.21}$$

$$H'_{22} = H_{22} + 2\theta H_{12}, \tag{4.22}$$

$$H'_{12} = H_{12} + \theta(H_{11} - H_{22}). \tag{4.23}$$

It is sufficient to only consider infinitesimal transformation as we will see. To proceed we examine the change of Eq.(4.18)

$$\Delta P = \frac{dp_{11}}{dH_{11}} \Delta H_{11} p_{22} p_{12} + \frac{dp_{22}}{dH_{22}} \Delta H_{22} p_{11} p_{12} + \frac{dp_{12}}{dH_{12}} \Delta H_{12} p_{11} p_{22}. \tag{4.24}$$

Inserting the infinitesimal expression for the rotation of the elements in H and noting that for example

$$\frac{dp_{11}}{dH_{11}} = p_{11} \frac{d \ln p_{11}}{dH_{11}} \tag{4.25}$$

we obtain the equality relation between before and after the rotation

$$P(H) = P(H) \left[1 - \theta \left(2H_{12} \frac{d \ln p_{11}}{dH_{11}} - 2H_{12} \frac{d \ln p_{22}}{dH_{22}} - (H_{11} - H_{22}) \frac{d \ln p_{12}}{dH_{12}} \right) \right]. \tag{4.26}$$

For the probability to be invariant under this transformation the second term in the bracket of the right hand side expression must be equal to zero

$$\frac{1}{2(H_{11} - H_{22})} \left(\frac{d \ln p_{11}}{dH_{11}} - \frac{d \ln p_{22}}{dH_{22}} \right) - \frac{1}{H_{12}} \frac{d \ln p_{12}}{dH_{12}} = 0. \tag{4.27}$$

This differential equation is easy to solve (the answers can be guessed), the results are

$$p_{11}(H_{11}) = e^{-AH_{11}^2 - BH_{11}}, \tag{4.28}$$

$$p_{22}(H_{22}) = e^{-AH_{22}^2 - BH_{22}}, \tag{4.29}$$

$$p_{12}(H_{12}) = e^{-2AH_{12}^2}, \tag{4.30}$$

with A and B positive constants. Combining these results with Eq.(4.18) and setting the energy offset $H_{11} + H_{22} = 0$ yields

$$P(H) = Ce^{-A\mathrm{Tr}(H^2)} \tag{4.31}$$

where C is a constant to be determine by the normalisation condition. The occurrence of the trace in Eq.(4.31) should come as no surprise as it is an invariant measurement of the Hamiltonian. Hence, it is invariant under any unitary transformation and is valid in any basis. This idea can be carried even further to define an invariant metric $(ds)^2$ which gives a measurement on the distance between Hamiltonians [36]. Eq.(4.31) is actually a general result that is valid for all three of the matrix ensembles, the difference being how the trace is evaluated.

To compare this result to our previous one Eq.(4.16), we have to change Eq.(4.31) to variables describing the energy-spacing. For this purpose we need the eigenvalues to the Hamiltonian matrix H, these are easily calculated to be

$$e_{\pm} = \frac{1}{2}(H_{11} + H_{22}) \pm \frac{1}{2}\sqrt{(H_{11} - H_{22})^2 + 4H_{12}^2}. \tag{4.32}$$

The connection between the two variable realisations are provided by a orthogonal transformation in such a way that the matrix is diagonalised $D_{\pm} = OHO^t$. The two representations are then related as

$$H_{11} = e_+ \cos^2(\phi) + e_- \sin^2(\phi) \tag{4.33}$$

$$H_{22} = e_+ \sin^2(\phi) + e_- \cos^2(\phi) \tag{4.34}$$

$$H_{12} = (e_+ + e_-) \sin(\phi) \cos(\phi). \tag{4.35}$$

With the knowledge how the variables are related we can calculate the Jacobian to determine how

$$P(H)dH \tag{4.36}$$

is transformed to

$$P(e_+, e_-, \phi)de_+de_-d\phi. \tag{4.37}$$

The Jacobian is given by

$$\det\left(\frac{\partial(H_{11}, H_{22}, H_{12})}{\partial(e_+, e_-, \phi)}\right) = e_+ - e_-. \tag{4.38}$$

Noting that $\mathrm{Tr}(H^2) = e_+^2 + e_-^2$ we have

$$P(e_+, e_-) = C(e_+ - e_-)e^{-A(e_+^2 + e_-^2)}. \tag{4.39}$$

Introducing the energy-spacing $s = e_+ - e_-$ and $z = \frac{1}{2}(e_+ + e_-)$ this can be expressed as

$$P(s, z) = Cse^{-A\frac{s^2}{2}}e^{-2Az^2}. \tag{4.40}$$

The dependence on z can be integrated out by noting that the resulting integral is a standard Gaussian

$$\int dze^{-2Az^2} = \sqrt{\frac{\pi}{2A}}, \tag{4.41}$$

and hence

$$P(s) = Cs\sqrt{\frac{\pi}{2A}}e^{-A\frac{s^2}{2}}. \tag{4.42}$$

To determine the constants C and A we use the normalisation condition mentioned before but also define what is known as the *mean-level spacing* (called D before), here we set this value equal to one to get

$$1 = \int_0^\infty dssP(s) = C\frac{\pi}{2A^2}. \tag{4.43}$$

Normalisation gives

$$1 = \int_0^\infty dsP(s) = \frac{2A}{\pi}, \tag{4.44}$$

resulting in $A = C = \pi/2$. Thus we finally obtain the level-spacing distribution corresponding to a random matrix

$$P_W(s) = \frac{\pi}{2}se^{-\frac{\pi}{4}s^2}. \tag{4.45}$$

This distribution is often called the *Wigner distribution* or the *Wigner surmise* (we will stick to the latter name to avoid mix up with the Wigner quasi-probability distribution used in the phase space formulation of quantum mechanics). This result was obtain under the assumption of only real elements in the Hamiltonian. When complex or quaternion numbers are contained in the Hamiltonians elements we have to considerer different transformations, such as unitary and symplectic. In large the resulting derivation are akin to the one we performed here which was orthogonal transformations. The results will not change to much either, the general form will still resemble a Gaussian, but with different width [3]. In figure (2) we can see both the Wigner surmise (for the case considered here) and the Poission distribution. From this we see that the Wigner surmise predicts zero probability for energy levels located at the same value. This means that the separation between levels are virtually always non-zero. This phenomena is called *level repulsion*. In contrast, the Poission distribution, which is characteristic for a system possessing regular dynamic, dictates that we have the direct opposite, levels tend to cluster together. The reason for this difference is what we discussed in the beginning of this section, degeneracy. It is known from perturbation theory [10] that states that are coupled will have energy-levels that repel each other. This is exactly what we expect would happen for strongly interacting systems where the number of constants of the motion are all but gone. Hence, the appearance of level repulsion is not that surprising and is an indication of non-integrable dynamic in the system. The presence of non-integrability is a necessary condition for chaos, even in the quantum world.

In this section we have omitted a large amount of theory considering random matrices and the connection to quantum chaos manifestations. Maybe most prominent is *unfolding of the spectra.* This method is necessary in order to compare measured spectrum with predictions. We are usually only interested in the local behaviour of the spectra and spacing. For more information about this subject and others see for example the given sources in the beginning of the section.

4.3.4 Quantum Thermalization (Eigenstate Thermalization Hypothesis)

Up until this point we have ignored the transition of a very important concept from classical mechanics into the quantum world. In section 4.1.2 we briefly discussed the subject of ergodicity and gave the fundamental definition as it is usually seen. We however refrained from mentioning why ergodicity is such an important concept. The equality of time and phase space average can of course be seen as a calculation aid but it has further implication then what could be seen at first. Most important, ergodicity implies the emergence of the microcanonical ensemble, the heart of all of equilibrium (and much of non-equilibrium) statistical mechanics [50]! Recall that the mircrocanonical ensemble at its essence describes systems with a given energy where every microstate (corresponding to a certain energy interval) is equally probable. If this is the case, the system is in thermal equilibrium (we considerer only an isolated system). This is something which follows naturally from ergodicity as an ergodic flow explore all of the available phase space. The question of which state a system is in are then slightly redundant as we know that the system will spend equal time in every part of phase space [50]. As a consequence, we assign every state equal probability. How does this play into chaos and integrability? The fact that statistical mechanics even can describe microscopic systems indeed rest on ergodicity. As is well known from introductory courses in statistical mechanics, the aim of the subject is not to explore the behaviour of individual particles but the system as a whole. It is, however, very likely that the underlying dynamics describing the interactions between the particles are complicated, especially if the number is high. As such this underlying dynamic is very likely to be non-integrable and furthermore, chaotic. Thereof the concept of ergodicity appears and it is exactly because of this that we can make predictions of the system by only considering "global" properties and not having to bother with details concerning individual particle-particle interactions.

Important to remember is that this formulation of statistical mechanics is a classical framework, that does not take into consideration quantum effects. Often the system are consisting of particles that correctly should be described quantum mechanically (or at least to a higher degree of accuracy). As often has been the case we again find ourself in the position where we cannot carry over a classical concept into the quantum realm. Where we preciously could ascribe the resulting ergodic behaviour as descending from the underlying chaotic dynamics we know that quantum mechanics lacks these properties, or at the very least manifest them in a different way. But if we lack chaos amongst the components then how can a system reach thermal equilibrium? Or more concretely, can a isolated quantum mechanical system, starting from an arbitrary initial state, reach a state that is akin to thermal equilibrium? The answer to the last question is actually already known from experimental results, the answer seems to be that an isolated quantum system (to a very high degree of accuracy) can exhibits thermal relaxation to thermal equilibrium [51]. The task now is to try and understand how this is possible from a theoretical viewpoint. The most prominent method to explain this is called *the eigenstate thermalization hypothesis* (ETH) [51, 52] and we will now outline some of the central arguments.

Our starting point is an isolated, non-integrable system in an arbitrary initial state. The time dependent state when expanded in energy eigenstates $|e_\alpha\rangle$ reads

$$|\psi(t)\rangle \sum_{\alpha=1}^{D} c_\alpha e^{-ie_\alpha t/\hbar} |e_\alpha\rangle \,. \tag{4.46}$$

As the system is non-integrable we do not have to worry about degenracies and can label the energy-eigenvalues according to increasing value. We are interested in the matrix elements of a given operator as a function of time

$$\langle\psi(t)| \hat{A} |\psi(t)\rangle = \sum_{\alpha,\beta}^{D} c_\alpha^* c_\beta A_{\alpha\beta} e^{-i(e_\alpha - e_\beta)t/\hbar}, \tag{4.47}$$

or more precisely, of its long-time behaviour. Defining the average of $\hat{A}$ in the long-time limit as

$$\overline{A} \equiv \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau \langle\psi(t)|\hat{A}|\psi(t)\rangle dt = \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau \sum_{\alpha,\beta}^{D} c_\alpha^* c_\beta A_{\alpha\beta} e^{-i(e_\alpha - e_\beta)t/\hbar} dt. \tag{4.48}$$

The integration of this expression is not to difficult. We separate the case $\alpha = \beta$ and then the remaining integration is straightforward

$$\overline{A} = \sum_{\alpha=1}^{D} |c_\alpha|^2 A_{\alpha\alpha} + i\hbar \lim_{\tau\to\infty} \left[\sum_{\alpha\neq\beta}^{D} \frac{c_\alpha^* c_\beta A_{\alpha\beta}}{e_\beta - e_\alpha} \left(\frac{e^{-i\left(e_\beta - e_\alpha\right)\tau/\hbar} - 1}{\tau} \right) \right]. \tag{4.49}$$

Taking the limit $\tau \to \infty$ in the second term yields zero provided that the phase factor in the exponential does not become to large[38]. Hence, we have for the long-time average of $\hat{A}$

$$\overline{A} = \sum_{\alpha=1}^{D} |c_\alpha|^2 A_{\alpha\alpha}, \tag{4.50}$$

which is known as the *diagonal ensemble* [51]. Eq.(4.50) still contains information related to the starting state characterised by the coefficients c_α in the α summation. It is therefore not the same as one would expect from the microcanonical ensemble which only depends on given global properties of the system. The microcanonical ensemble long-time average for the same operator $\hat{A}$ is given by [51]

$$\langle A \rangle_{\text{mc}} = \frac{1}{\mathcal{N}} \sum_{\gamma=1}^{\mathcal{N}} A_{\gamma\gamma} \tag{4.51}$$

where $\mathcal{N}$ is the number of states in the appropriate energy window and γ is constrained to states contained in this energy window. Eq.(4.51) only relates to properties of the system and not to any initial state (apart from the system energy). The statement that relaxation to thermal equilibrium takes place in quantum system corresponds to the validity of Eq.(4.51) in describing the long-time behaviour of observables. The question now is how both Eq.(4.50) and Eq.(4.51) both can be valid in the same theoretical framework. There are no uniformly agreed upon explanation on how and why this is the case. The most common way to reconcile these two long-time ensemble averages is as follows (and it is this that constitute the ETH). If we where to assume that $A_{\alpha\alpha}$ in Eq.(4.50) fluctuate very little or nothing between energy-states, provided they are close in energy, then we can move this term out of the summation. If this is the case then for normalised initial states

$$\overline{A} = \sum_{\alpha=1}^{D} |c_\alpha|^2 A_{\alpha\alpha} \approx A \sum_{\alpha=1}^{D} |c_\alpha|^2 = A, \tag{4.52}$$

where $A = A_{\alpha\alpha}$. The occurrence of the initial state structure amounts to unity for an arbitrary normalised starting state. At the same time, this assumption also affect Eq.(4.51) such as

$$\langle A \rangle_{\text{mc}} = \frac{1}{\mathcal{N}} \sum_{\gamma=1}^{\mathcal{N}} A_{\gamma\gamma} \approx \frac{1}{\mathcal{N}} \sum_{\gamma=1}^{\mathcal{N}} A = A, \tag{4.53}$$

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[38] For this to always be the case we have to assume non-integrability (random eigen-energyvalues). Otherwise we could have the case where the phase factors happens to be for some t identical meaning the limit does not necessarily have to go to zero (as we have an infinite number of complex terms this could happen). But if $\overline{A}$ is to be time-independent we must have that the limit goes to zero.

where the result follows from the assumption that all the $A_{\gamma\gamma}$ are the same in the energy window. The conclusion is that under this assumption both ensembles predict the same result for the expectation value of an observable. Where in the classical case a starting state is through out time-evolution “forced” into a thermal state, a quantum state starts out in a superposition of energy-eigenstates where the final thermal state is contained but hidden by the occurrence of coherence. As the initial state evolves in time this coherence disappear and the final thermal state emerge[39]. In the same way that ergodicity is a necessary tool to explain the validity of statistical mechanics, so is the Eigenstate Thermalization Hypothesis used to justify quantum statistical mechanics. Important to note is that other arguments can be made to arrive at the same conclusion. Yet, ETH is the often preferred explanation for various reasons [52].

Important to keep in mind is that not all closed quantum systems thermalize according to this procedure. Systems that are integrable will not thermalize. Hence, only non-integrable systems thermalize (which is not to strange seeing how we assume chaotic behaviour when motivating ergodicity in classical statistical mechanics). The problem is that we do not have any clear definition of non-integrable systems in quantum mechanics. The result is that some systems which appears to be non-integrable fails to thermalize. Again, the quantum world fails to adhere to explanations taken directly from the classical realm.

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[39] The result of thermalizing is that the reduced density matrix is thermal in the sense that it maximise the amount of entropy.

Part III

Calculations, Results and Analysis

“I pass with relief from the tossing sea of Cause and Theory to the firm ground of Result and Fact.” - Winston S. Churchill

5 Problem set-up

In this section we will discuss the system under consideration and motivate why this model is a good choice for examining the phenomena which we are interested in. Some of this are reiterating what we mentioned in the introduction (albeit in a slightly more detail fashion).

As hinted at in the introduction we want to examine the affect on a chaotic system due to its interaction with an environment. We now restate this query in more detail. With a chaotic quantum system we mean one which exhibits tendencies according to one of the methods outlined in section 4.3.2. The most commonly employed is the one which stem from random matrix theory which impose predictions on the energy level statistics. A chaotic system will exhibit a Wigner surmise/distribution of the spacing between energy-levels. In addition, we expect some elements of classical chaos to be present, even in the cases where a classical correspondence to the system is undefined. Most prominent is the concept of ergodicity which we expect will also be present in the phase space distribution for a quantum system[40]. Aside from the classical correspondence (when possible) we also expect this to be true as a consequence of the eigenstate thermalization hypothesis. Given any initial state $\rho(0)$, it would not be inconceivable that as a consequence of the underlying chaotic dynamic, it evolves to a thermal state in accordance to section 4.3.4. A thermal state is one which maximise the entropy (exhibiting as large amount of entanglement as possible given the symmetry constrains) [10, 53] and as a consequence spread out in phase space. Connected to this is the belief that a chaotic quantum system always thermalizes (even though this have not been proven and there seems to be some exceptions [54, 55]). Thus, we expect that a chaotic quantum system will explore a larger part of phase space (spread out in phase space) than a non chaotic system. Furthermore, we also know that the interaction of a closed quantum system with an environment introduces decoherence. But for a chaotic quantum system, the classical limit which is induced by decoherence should be an ergodic classical chaotic system. Therefore, a plausible assumption would be that the interaction of a chaotic quantum system with an environment should result in a quicker spread of the phase space distribution compared to a closed one, as the interaction with the environment promotes decoherence, i.e. mixedness. Moreover, we also reckon that the interaction of a system with a thermal environment would speed up the process of quantum thermilzation, causing the system to thermilize quicker. There are, however, reasons to believe that this is not the case [56]. It appears that the spreading in phase space is delayed, suggesting that an open quantum system should thermilaze slower

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[40] Even though the direct interpretation is complicated. In a strict sense it is hard to define quantum ergodicity [57].

then a closed. The reason for this is again decoherence. On short time scales quantum and classical predictions approximately coincide (by virtue of the Ehrenfest theorem) [45, 56], which can be seen from the Fokker-Planck equation (equation of motion for the quasi-probability distribution). A connection with an environment causes a system's expectation values to longer match up between quantum and classical versions [58]. Accordingly, decoherence induced by this connection makes the distribution localised longer. This may appear to be in conflict to what was said above about decoherence hastening the spread out in phase space. Yet, this is not directly a contradiction as these two behaviours are on different time scales. For short times decoherence tends to localize the distribution more, while in the long time limit decoherence forces the distribution to spread[41]. This initial localisation is in contrast to what we would conjecture with respect to quantum thermalization: Can a bath delay thermalization? It is this counter-intuitive phenomena which we will examine.

One system that exhibits signatures of quantum chaos is the one described by the *Dicke Hamiltonian* [59]. In appendix A.1 we present a derivation of the Dicke Hamiltonian. The reader unfamiliar with this Hamiltonian is encouraged to read that section first before continuing the current one. In its essence, the Dicke Hamiltonian describes the interaction between two-level atoms and a quantized electromagnetic field. Hence, it is a general system which is realisable in a laboratory setting [60]. In addition, it represents a system which from a theoretical viewpoint is not to complicated. For an environment we choose again an electromagnetic field. We will also consider the case where decoherence is caused by a "measurement" performed by the environment. With these specifications we can derive the corresponding master equation. However, in this thesis we will instead consider a master equation on the form [61] (with $\hbar = 1$)

$$\frac{d}{dt}\rho(t) = -i\left[H_D, \rho(t)\right] - \frac{1}{2}\kappa\left(a^\dagger a\rho(t) + \rho(t)a^\dagger a - 2a\rho(t)a^\dagger\right), \tag{5.1}$$

with

$$H_D = \omega a^\dagger a + \omega_0 S_z + \frac{g}{\sqrt{j}}(a^\dagger + a)(S_+ + S_-) \tag{5.2}$$

the Dicke Hamiltonian[42] restricted to one mode of the electromagnetic field (compare with Eq.(A.25)). Eq.(5.1) is given in the Lindblad form (compare with Eq.(3.31)),

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[41] Remember the fact that the classical limit of a quantum state is a Liouville distribution which exhibit chaos by "stretching and folding". In turn this is related to the concept of mixing (which is the more formal way of defining chaos for a distribution). A quantum distribution cannot exhibit this feature. If decoherence is the cause for the transition from quantum to classical behaviour then it must aid the development of ergodicity as it is connected to the mixing property. This must, however, only be true in the long time limit (recall the definition of ergodicity).

[42] Compared to the form presented in appendix A.1 the coefficient in front of the third term is different. Aside from a name change to the more conventional g from ϵ we have also divided by $\sqrt{j}$ which

where the Lindblad operator is $L = a$ (for the case of measuring we will take the Lindblad operator on the form $L = x$). Therefore Eq.(5.1) represents losses (dissipation) of photons from the system into the environment. The amount of losses is regulated by the system-interaction parameter κ, where a larger κ induces more losses.

Before we stated Eq.(5.1), we said that a derivation of the master equation was possible from the specification of the system and environment. If this derivation is carried out, is the result the same as the one in Eq.(5.1)? The answer is obviously no as the Lindblad operator on the form $L = a$ is restricted to a set-up where the system is a harmonic oscillator interacting with an environment of harmonic oscillators. Even more, we can see that the Dicke Hamiltonian contains two kinds of system operators, representing the electromagnetic field as-well as the two-level atoms. These pseudo-spin operators must in a correct derivation of the master equation be coupled to the electromagnetic field of the environment in some way (that is to say the Lindblad operators would contain a reference to S_z and/or S_x). As a consequence of this, in the long time limit the system will not relax to the vacuum state despite coupling to a zero temperature photon bath. Hence, we can think of Eq.(5.1) as describing a system which is not in equilibrium with the environment, or that it is driven out of equilibrium with the environment. This last point actually has some merit. In order for the Dicke Hamiltonian to exhibit chaos we must be in a certain parameter range (more on that later). These parameter values will in turn render some of the assumptions made when deriving the Dicke Hamiltonian invalid. Yet, it is possible to evade this. In order to achieve this in the laboratory, an applied laser must be used to transform our two-level atoms to a third level. This third state is, however, only virtually populated because it is assumed off resonant from the applied fields. The result of this is that we obtain an effective coupling between the two initial states [62], keeping the overall structure of the Dicke Hamiltonian. Why we do not see the presence of any time-dependent driving term in the Hamiltonian is because of a cleaver change of frame to a rotating one where the Hamiltonian is time-independent. When we are in this parameter range the form of the master equation, Eq.(5.1) is valid (or at the very least an excellent approximation). Together with this, the fact that Eq.(5.1) is simpler than the correspondingly "correct" derived master equation makes it the better choice for this thesis.

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is defined in the way that $j = \frac{Number\ of\ atoms}{2}$. The reason for this is to make the thermodynamic limit defined for all terms in the Hamiltonian [67].

6 Derivation of the Fokker-Planck Equation

In the previous section we presented the master equation which is our starting point in this thesis. From chapter 2 we know that the Wigner or Husimi function also contains the same information as the density operator, and furthermore that the corresponding equation of motion is possible to state. Here we will derive an equation of motion for the Husimi function starting from Eq.(5.1). The derivation will not be complete as to keep the length of the thesis in check, and therefore when necessary reference will be given instead. This type of equation describes the time-evolution of a (quasi) probability distribution is know as a *Fokker-Planck Equation.* Important to stress is that it is possible to derive a Fokker-Planck equation starting from Eq.(2.79), therefore making no reference whatsoever to the operator formalism. The problem with this approach is that we have to deal with the phase space representation of spin operators which is not always an easy task. In this case at least it is easier to start from the operator formalism and transform it to phase space. With that said, it would be satisfactory from a purely theoretical self-contained view to derive the Fokker-Planck equation without making any reference to the operator formalism.

Starting by multiplying[43] both sides of Eq.(5.1) with $\langle \alpha, z|$ from the left and $|\alpha, z\rangle$ from the right (can also be thought as constructing the matrix element in the αz basis from the density operator) we get

$$\langle \alpha, z| \frac{d}{dt}\rho(t) |\alpha, z\rangle = \langle \alpha, z| -i\left[H_D, \rho(t)\right] |\alpha, z\rangle - \langle \alpha, z| \frac{1}{2}\kappa \left(a^\dagger a\rho(t) + \rho(t)a^\dagger a - 2a\rho(t)a^\dagger\right) |\alpha, z\rangle . \tag{6.1}$$

From this we want to construct the phase space analogy to the operators $a^\dagger$, a, S_z, S_+ and S_-. First we consider the second term (the one stemming from the connection of the system with an environment), as it only contains creation and annihilation operators

$$- \langle \alpha, z| \frac{1}{2}\kappa \left(a^\dagger a\rho(t) + \rho(t)a^\dagger a - 2a\rho(t)a^\dagger\right) |\alpha, z\rangle . \tag{6.2}$$

The canonical and spin coherent states can be written as a product state $|\alpha, z\rangle = |\alpha\rangle |z\rangle$, this allow us to disregard any affect of the creation and annihilation operators on the spin coherent states (they live in different spaces). For the first term we have that $\langle\alpha| a^\dagger = \langle\alpha| \alpha^*$, as α^* is the eigenvalue to the operator $\alpha^\dagger$, see section 2.5. The case of $\langle\alpha| a$ requires a bit more thought. Instead of this form we can consider $a^\dagger |\alpha\rangle$ which is

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[43] Strictly, in principle we have to also multiple with normalisation factors included in the definition of the Q function. But as we do this on both sides and then included them when we define $Q(\alpha, z)$ they serve no calculation purpose. Thus, we will omit them here, even though it should be kept in mind that they in some sense are there.

the hermitian conjugate of the present case. Writing the coherent state in the number basis we have that

$$a^\dagger |\alpha\rangle = a^\dagger \left(e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \right), \tag{6.3}$$

recalling the effect of $a^\dagger$ on a number state $|n\rangle$ [10] this becomes

$$\left(e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \sqrt{n+1} \, |n+1\rangle \right). \tag{6.4}$$

Defining $m = n + 1$ this reads

$$a^\dagger |\alpha\rangle = \left(e^{-|\alpha|^2/2} \sum_{m=1}^{\infty} \frac{\alpha^{m-1}}{\sqrt{m-1!}} \sqrt{m} \, |m\rangle \right). \tag{6.5}$$

But this looks almost the same as what we would get if we acted with a derivative on the state $|\alpha\rangle$, such as

$$\begin{aligned} \frac{\partial}{\partial\alpha} |\alpha\rangle = \frac{\partial}{\partial\alpha} \left(e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \right) &= -\frac{\alpha^*}{2} e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle + e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} n \frac{\alpha^{n-1}}{\sqrt{n!}} |n\rangle \\ &= -\frac{\alpha^*}{2} |\alpha\rangle + e^{-|\alpha|^2/2} \sum_{n=1}^{\infty} \sqrt{n} \, \frac{\alpha^{n-1}}{\sqrt{n-1!}} |n\rangle = -\frac{\alpha^*}{2} |\alpha\rangle + a^\dagger |\alpha\rangle, \end{aligned} \tag{6.6}$$

where we in the next to last step changed the summation to take into consideration that the factorial of a negative number times zero is undefined. With this we can write the creation operator as a differential operator

$$a^\dagger |\alpha\rangle = \left(\frac{\partial}{\partial\alpha} + \frac{\alpha^*}{2} \right) |\alpha\rangle. \tag{6.7}$$

The reader may recognise this form, this is nothing else than the Bopp operators encountered earlier in section 2.3.5, but expressed in terms of creation and annihilation operators (complex numbers). In this case, using purely phase space methods could be considered an option, which is not more demanding than the operator formalism. For consistency reasons we opted not to use it here however. With this we can easy obtain the result for $\langle\alpha| a$ by taking the hermitian conjugate. Hence, we have that

$$\frac{1}{2}\kappa \langle \alpha, z| a^\dagger a = \frac{1}{2}\kappa \langle \alpha, z| \alpha^* \left(\frac{\partial}{\partial\alpha^*} + \frac{\alpha}{2} \right), \tag{6.8}$$

and for the entire term

$$\frac{1}{2}\kappa \langle \alpha, z| \, a^{\dagger} a \rho \, |\alpha, z\rangle = \frac{1}{2}\kappa \langle \alpha, z| \, \alpha^{*} \left(\frac{\partial}{\partial \alpha^{*}} + \frac{\alpha}{2} \right) \rho \, |\alpha, z\rangle . \tag{6.9}$$

We want to move the derivative outside of the bra-ket expression. If we are to do this we have to keep in mind that the derivative is suppose to act to the right, meaning that if we move it out we will obtain an extra term (because both the bra and ket contains reference to $|\alpha|^2$). This is easily amended by adding an additional term consisting of $\frac{\alpha}{2}$ (which is the result of the derivative acting on the exponential term in expression for the coherent state). Doing this we are left with

$$\frac{1}{2}\kappa \langle \alpha, z| \, a^{\dagger} a \rho \, |\alpha, z\rangle = \frac{1}{2}\kappa \alpha^{*} \left(\frac{\partial}{\partial \alpha^{*}} + \alpha \right) \langle \alpha, z| \, \rho \, |\alpha, z\rangle = \frac{1}{2}\kappa \alpha^{*} \left(\frac{\partial}{\partial \alpha^{*}} + \alpha \right) Q(\alpha, z), \tag{6.10}$$

where in the last step we used the definition (again omitting any relevant factors) of the joint Husimi Q function for canonical and spin-coherent states [27]

$$Q(\alpha, z) = \langle \alpha, z| \, \rho \, |\alpha, z\rangle . \tag{6.11}$$

In a very similar manner we can obtain the phase space representation for the remaining terms stemming from the environment connection. The result is

$$\begin{aligned} &- \langle \alpha, z| \, \frac{1}{2}\kappa \left(a^{\dagger} a \rho(t) + \rho(t) a^{\dagger} a - 2 a \rho(t) a^{\dagger} \right) |\alpha, z\rangle = \\ &= -\frac{1}{2}\kappa \left(\frac{\partial}{\partial \alpha} \alpha + \alpha^{*} \frac{\partial}{\partial \alpha^{*}} - 2 \frac{\partial}{\partial \alpha^{*}} \alpha^{*} - 2\alpha \frac{\partial}{\partial \alpha} - 2 \frac{\partial}{\partial \alpha} \frac{\partial}{\partial \alpha^{*}} \right) Q(\alpha, z) = \mathcal{L}_{relax} Q(\alpha, z), \end{aligned} \tag{6.12}$$

where we in the last step introduced the phase space relaxation differential operator $\mathcal{L}_{relax}$. This expression tells how the environment affects the time-evolution of $Q(\alpha, z)$.

With the environment term out of the way we shift our focus to the term containing the commutator. Writing it out explicitly we have

$$-i \langle \alpha, z| \, H_D \rho \, |\alpha, z\rangle + i \langle \alpha, z| \, \rho H_D \, |\alpha, z\rangle . \tag{6.13}$$

It is enough to only calculate one of these terms as the other only differ by a hermitian conjugate. Picking the second term and writing out the Hamiltonian yields

$$i \langle \alpha, z| \, \rho H_D \, |\alpha, z\rangle = i \langle \alpha, z| \, \rho \left(\omega a^{\dagger} a + \omega_0 S_z + \frac{g}{\sqrt{j}} (a^{\dagger} + a)(S_{+} + S_{-}) \right) |\alpha, z\rangle . \tag{6.14}$$

The first term from the Hamiltonian is trivial, we just use the same method as when we calculated the environment terms. The other two are more interesting as they contains pseudo-spin operators. We will only calculate the correspondence for one of the operators, to demonstrate the approach. Overall the procedure is akin to that for the canonical coherent state and the creation/annihilation operators, although some complications are unavoidable. For the rest of the operator correspondences see [59]. Taking S_- as the example, we have that it only acts on the spin coherent state. Using the form given in section 2.5.2, and the notion that the phase space representation of a ladder operator can be realised as a differential operator (inspired by the canonical coherent state situation considered previously), we examine the effect of the derivative on a spin coherent state

$$\begin{aligned}\frac{\partial}{\partial z}\left|z\right\rangle = \frac{\partial}{\partial z}\left(\frac{1}{(1+|z|^2)^j}e^{zS_-}\left|j,j\right\rangle\right) &= -\frac{jz^*}{(1+|z|^2)^{j-1}}e^{zS_-}\left|j,j\right\rangle + S_-\frac{1}{(1+|z|^2)^j}e^{zS_-}\left|j,j\right\rangle \\ &= -\frac{jz^*}{(1+|z|^2)}\left|z\right\rangle + S_-\left|z\right\rangle .\end{aligned} \tag{6.15}$$

From this we can conclude that

$$S_-\left|z\right\rangle = \left(\frac{\partial}{\partial z} + \frac{jz^*}{(1+|z|^2)}\right)\left|z\right\rangle . \tag{6.16}$$

For this spin operator the result was easy to obtain. The remain two cases are, however, a bit more difficult.Here we only state the results and refer to Ref. [59] for the interested reader. With these results, and the one we obtained for the extra environment term, we get the Fokker-Planck equation for our total system

$$\dot{Q}(\alpha, z) = \left(\mathcal{L} + \mathcal{L}_{diff} + \mathcal{L}_{relax}\right) Q(\alpha, z), \tag{6.17}$$

with $\mathcal{L}_{relax}$ as given in Eq.(6.12), and

$$\mathcal{L} = i\frac{\partial}{\partial \alpha}\left(\omega\alpha + \frac{g}{\sqrt{j}}(j+1)\frac{z+z^*}{1+|z|^2}\right) + i\frac{\partial}{\partial z}\left(-\omega_0 z + \frac{g}{2\sqrt{j}}(1-z^2)(\alpha+\alpha^*)\right) + c.c., \tag{6.18}$$

$$\mathcal{L}_{diff} = i\frac{g}{\sqrt{j}}\frac{\partial^2}{\partial\alpha\partial z}(1-z^2) + c.c., \tag{6.19}$$

where "c.c." denotes complex conjugate with respect to the given terms. We see that the resulting Fokker-Planck equation consists of three parts originating from different sources. The first term, $\mathcal{L}$, is a term which is purely classical. This can be seen by recalling that it came from the two first terms in the Hamiltonian. Even though we are working in a unit system where $\hbar = 1$, we can see from the appendix that the two first terms in the Hamiltonian contains $\hbar$. The master equation in turn can be expressed (a bit haphazardly) as the von Neuman equation for the density matrix plus corrections. Hence, the first part of the master equation corresponding to unitary time-evolution is divided by $\hbar$. This factor will eliminate the one which is present in the first two parts of the Hamiltonian, meaning that we are left with terms containing no reference to $\hbar$. Therefore, we speak of a classical part which is unmodified in the classical limit $\hbar \to 0$. In contrast, $\mathcal{L}_{diff}$ do contain $\hbar$ (recall how the parameter in front of the third term in the Hamiltonian was defined) and we can picture this term as a quantum mechanical correction added to the first term representing classical flow in phase space. It is interesting to not the specific form of L_{diff} as a second order derivative. Such terms typically represent diffusion in flow equations. Indeed, this term is responsible for the absence of sub-Planck structures in the Husimi distribution; when the distribution gets very squeezed the "quantum preasure" (diffusion) gets dominant. Lastly, the relaxation term $\mathcal{L}_{relax}$ which where derived from the environment coupling is also a classical contribution. This should be no surprise because nothing in the system-enviornment coupling is unique to quantum mechanics in this case (it is possible to think about a classical system interacting with electromagnetic radiation described by waves). The classical limit of an open quantum system should be an open classical system, therefore the environment term should contain no reference to $\hbar$ (provided the system has a classical analogy).

If we were to considerer another environment, then we would only need to change the third term in Eq.(6.17). Luckily the other cases studied in this thesis, where the Lindblad operators represent measurement performed by the environment on the system, are represented by $L = x$ or $L = p$. Both of these can of course be written as creation and annihilation operators meaning that we can just repeat the derivation we performed above applied to this situation.

7 Methods of Calculations

With the equations of motion known we have come to the point where the task is to try and solve it. Keeping in mind that we consider a chaotic model it is self-evident that we cannot hope to solve the equations analytically. Instead we resort to numerical methods to give insight into the time-evolution of the phase space (quasi) distribution.

Here we have two options for attacking the problem. Either we solve the master equation and then transform the resulting density operator into a phase space distribution (utilising the methods given in chapter 2), or we solve the Fokker-Planck equation to directly obtain the time-evolved distribution. The question of which of these methods is used comes down to what is easiest to implement numerically, and what requires the least amount of computation power/time.

The Fokker-Planck equation is a partial differential equation, which in our case depends on four variables. Methods to solve a four dimensional partial differential equation exist, but are not always easy to implement. In addition, these methods can many times be demanding with respect to computational power.

The master equation is an operator valued equation. As can be suspected there exist an array of methods to solve and/or at least approximately solve a master equation. Some are more complicated than others and the required computational power varies. Depending on the nature of the problem, some are more appropriate than others for different situations. In this thesis we will use *the quantum jump method* (also know as *Monte Carlo wave-function method*). In appendix A.2 we present the general idea and discuss the method in some detail. What is most important is that it is equivalent with the master equation. Instead of considering a density operator which evolves under the influence of the system dynamics and environment, the quantum jump method takes a different approach and examine the behaviour of a collection of wave functions. Each wave function evolves according to an non-unitary Hamiltonian. The fluctuations (decoherence) induced by the environment is captured by introducing the possibility of stochastic quantum jumps at each time. Whenever or not a jump takes place is decided by comparing a randomly generated number (this is where the stochastic factor enters) with the product of the interaction strength, Lindblad operator and time step. In order for this procedure to be equivalent with the master equation formalism we must repeat this process many times (this is where the name Monte Carlo comes from regarding this method). Formally the amount of times we repeat this should be infinity. This is of course something which cannot be achieved in practice. Therefore, when implementing this method it is important to check that a sufficiently large amount of simulations are run to ensure that the behaviour does not differ from the corresponding master equation. Since we do not have access to the exact solution of the master equations, one checks the accuracy by checking convergence of the results; increasing the number of Monte Carlo simulations should not alter the results. It is this truncation of number of simulations that constitute the approximation in this method, usually a number of simulations can be reached which ensures that this method is an excellent approximation.

In order to ensure that the Dicke Hamiltonian exhibits chaos we must choose parameters related in such a way [5] that

$$g \geq \sqrt{\omega_0 \omega}. \tag{7.1}$$

It is also known that a large amount of particles (which determines the highest allowed value for the total pseudo spin in the z-direction) is required for chaotic behaviour to set in. Both of these conditions are checked to be satisfied to such a large extent as possible with the available computational power.

In order to perform these calculations we first diagonalize the Hamiltonian by writing it in a *bare basis* [64]. With this we mean a basis which at the start can be split up into a photon part (describe by the usual states in Fock-space) and a pseudo-spin part (described by the known spin eigenstates of S_z). Furthermore, the number of photons are truncated at a certain number. This is most apparent from how a coherent state is constructed (see chapter 2). This truncation will affect the results in the way that the detailed long time behaviour becomes muddle. Still, the overall results (especially for short times) should not be affected by this truncation.

8 Results and Analysis

In this section we will present the results from the numerical solution of the master equation, for the different cases of environments; photon losses or "position/momentum" measurement. All parameters will be given without units, i.e. we set $\hbar = 1$.. Important to stress is the fact that some of these results only applies to the bosonic part of the system[44]. The reason for eliminating the information about the spin is two-folded. First, we cannot visualise a four dimensional distribution in any easy way, meaning that the results are harder to interpret. Secondly (and more importantly), the required calculations for the spin part is often more obscure, the reason for why we will discuss a bit more in context later.

8.1 Photon-bath

In figures 3-5 the Husimi Q-function is presented for three different cases of coupling strengths κ. In the first plot, figure 3, the system is closed and we see a rather large spreading. The distribution is relatively irregular even though the structure of two distinct peaks is evident. These derive from the specific atom-ligt coupling [63]. For the

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[44] When solving the master equation by the quantum jump method we obtain a density matrix containing information about both the bosonic part and the spin part. By performing a partial trace (see section 3.1) we get the reduced density matrix for the bosons only.

following two figures, 4 and 5, the coupling to the environment has been included. The environment has the effect of smoothening the distribution which can be understood from the Fokker-Planck equation Eq.(6.17) where we saw that the bath adds a diffusion-like term. An additional effect is a narrower distribution. This is a result from the fact that the effective phase space volume is decreased when coupled to the environement.

Figure 6 illustrates how the width of the distribution evolves in time. It is in the context of figure 6 we see that the analogy for the spin part is not as straightforward as one can imagine. The variance of $\hat{x}$ and $\hat{p}$ is well defined in phase space, in the sense that we can parametrise these by the phase space coordinates x and p. From the product of these variances we construct a measurement on how broad the distribution is. If we where to repeat this process for the spin part we quickly see what the hurdle is. Where in the bosonic part we worked with $\hat{x}$ and $\hat{p}$, both of which have classical phase space counterparts in x and p, we know that for spin this is not the case. The parametrisation of spin requires the geometry of a sphere. Hence, if we want to relate the variance to the width of a distribution in phase space, we have to know how the angles θ and ϕ are related to the variances of S_x, S_y and S_z, which is not a trivial matter. Again, we see that the problem of describing spin in phase space can be traced back to the fact of the more complicated geometry compared to the bosonic case which correspond to a trivially flat space.

In figure 7 we present the expectation value of the number of photons. This is of relevance for the determination of steady-state, when the average fluctuate around a set value occurs.

The energy of the system state $\hat{\rho}(t)$ is shown in figure 8. As is clear, by increasing the coupling κ the energy is lowered. Roughly, this is an outcome of loss of photons to the environment. However, it should be remembered that the full picture is more complicated; the spin and boson field are coupled and the steady state of the system is one were the photon loss is in a sense balanced by gain from the coupling to the spin - the spin acts as a photon pump. The lowered system energy is also an indication that the effective phase volume becomes smaller, as discussed above for figure 6. It is also known that the two peaks seen in the distributions, figures 3-5, are more pronounced for low energies [63].

Finally, figure 9 gives the norm of the spin, $\hat{S}^2$. As explained in the caption, for the closed system the drop in $\hat{S}^2$ is an indication of atom-photon entanglement. The situation is not as trivial for the open case since then this quantity cannot distinguish “mixedness” arising from coupling to the environment or to the photon subsystem. Nevertheless, the plot makes clear that the bath adds more mixedness to the spin than what is just coming from the atom-photon entanglement.

In common for all the results is the initial state, which is taken to be a bosonic coherent state and a spin state where $m_{z=1/2}$. More precise we take

$$|\psi_{initial}\rangle = |\alpha\rangle \otimes \left|\psi_{m_z=1/2}\right\rangle , \tag{8.1}$$

as the initial state to be propagated in time, where $\left|\psi_{m_z=1/2}\right\rangle$ is a spin state where the expectation value of S_z is equal to 1/2. The reasons for this choice is that a coherent state is a localised minimum uncertainty state which can be considered the closest thing to a classical state we can formulate in quantum mechanics. The addition of this specific spin state is a bit arbitrary. Why we choose this was to aid in the development of chaos for the isolated system model. Furthermore, it is probable that a real physical system starts with at least some of the atoms excited following the construction of the system in the laboratory.

A remark concerning figure 3 is in place. It is known from examinations of the Dicke Hamiltonian that it exhibits quantum chaos[45]. Yet, we had problems achieving chaos to such an extent that the distribution uniformly spread out in the allowed phase space. It is possible that even larger systems and parameters are needed to see such kind of ergodic behaviour. These two are related, meaning that we cannot increase the values of the parameters without adjusting the size of the system. With the available computational power we are limited to the result in 3. Still, tendencies of the distribution to behave ergodic can be seen.

Let us now return to our original question: Will a coupling to the environment speed up or slow down the thermalization? On the one hand it is natural to expect the thermalization to occur more rapid if the system is in contact with a bath; both the internal and external (environmental driven) mechanism should strive after reaching a thermal state. However, we also argued that decoherence can act as a localization of the phase space for short times [56] which suggests that ergodicity (and thereby thermalization) is delayed. Now, judging from figure 6 we actually find that the characteristic time for thermalization (once the broadening has settled) does not seem to depend much on the coupling κ. We see that the spreading is slower for increasing κ but at the same time is the effective phase space volume decreased such that the ergodicity occurs roughly after the same time in all cases.

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[45] In most of these sources the energy-level spacing where examined. This is in contrast to what we are trying to examine here which is the ergodic behaviour implied by this chaotic dynamic.

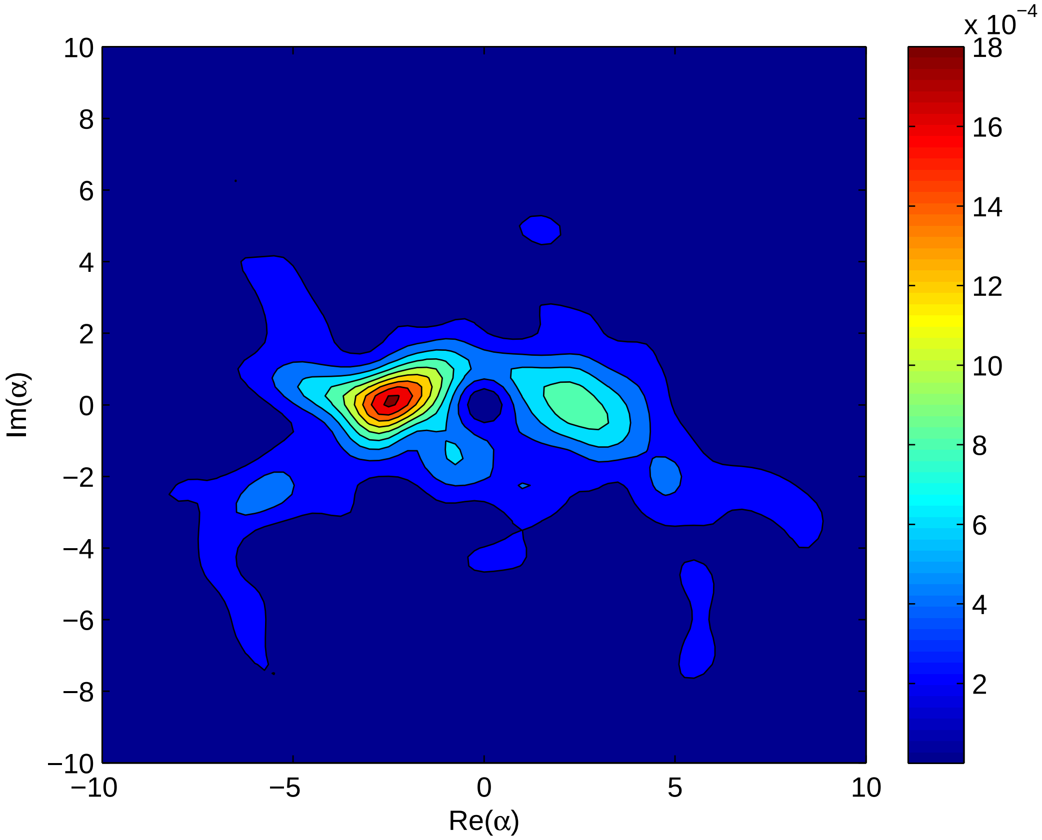

Figure 3: A contour plot of the quasi-probability distribution $Q(\alpha)$ for the environment coupling coefficient $\kappa = 0$ (at t=10). The system specific values of the parameters are $\omega = \omega_0 = 1$, $g = 2$, the number of photons (photon truncation) $n = 100$, the number of two-level atoms $N = 20$ which set the total spin to $j = \frac{N}{2} = 10$. The number of Monte Carlo simulations is $M = 2000$. The final propagation time is $t = 10$ and the size of the time steps where $dt = 0.010$. This figure corresponds to the case of an isolated system described by the Dicke Hamiltonian. Note the spread of the distribution which is an indication of the chaotic dynamics underlying the Dicke system. The concept of ergodicity is not totally lost in the quantum realm.

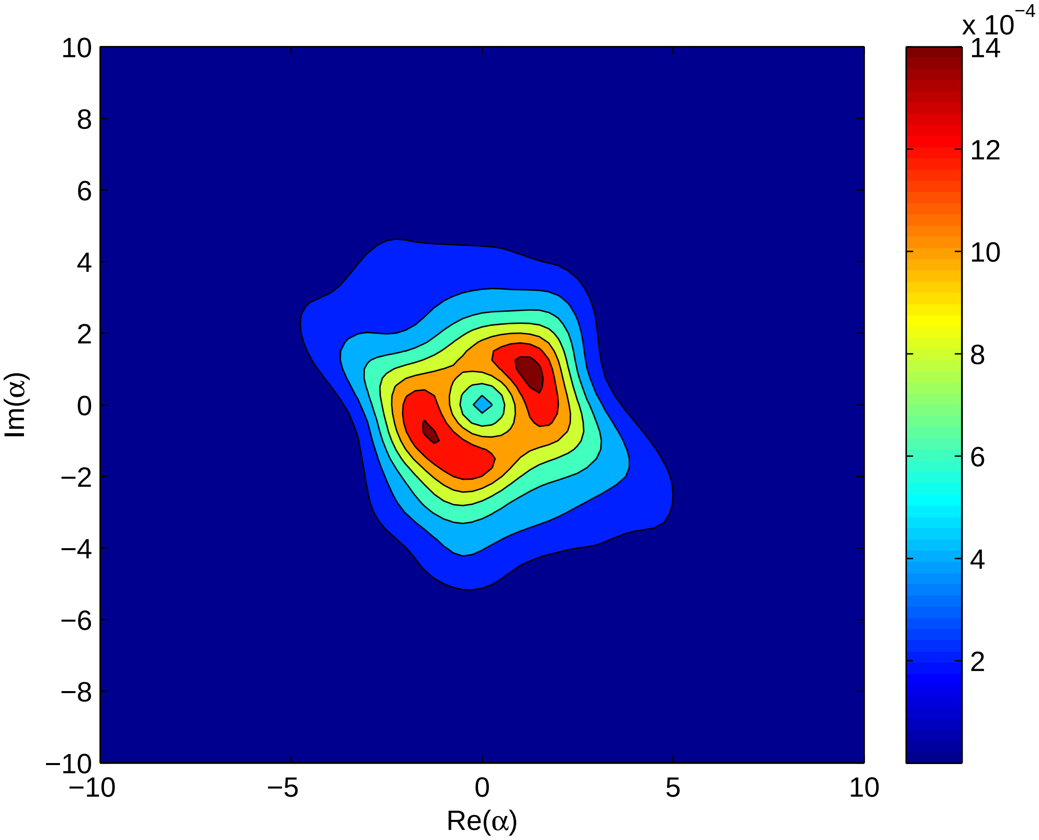

Figure 4: A contour plot of the quasi-probability distribution $Q(\alpha)$ for the environment coupling coefficient $\kappa = 0.06$ (at t=10). The system specific parameters are the same as in figure 3. With the introduction of a non-zero coupling to the environment we see that the distribution appears more localised. In addition, a rotation has taken place compared to the $\kappa = 0$ case. This is caused by the presence of the environment which modifies the original Hamiltonian for the isolated system, a so called *Lamb shift* [61].

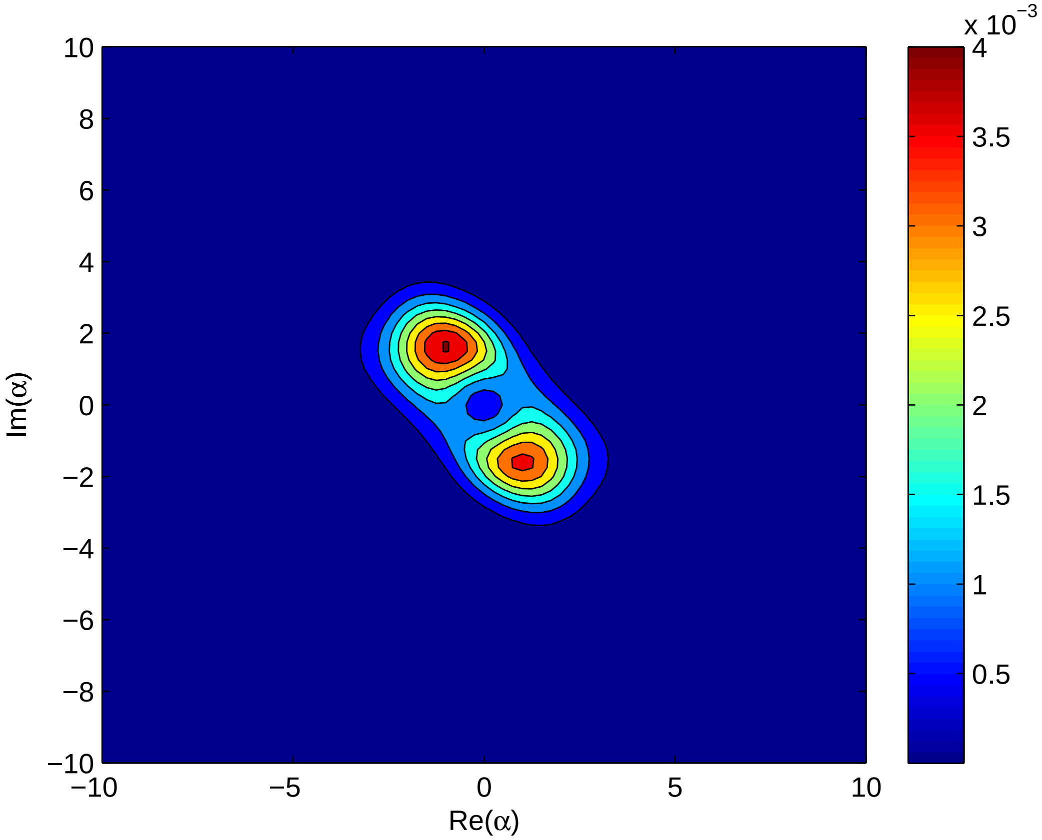

Figure 5: A contour plot of the quasi-probability distribution $Q(\alpha)$ for the environment coupling coefficient $\kappa = 0.6$ (at t=10). The system specific parameters are the same as in figure 3. With a stronger coupling the distribution still shows sign of being more localised then figure 3. Yet, compared to figure 4 additional structure has emerged. Two visually distinct areas are prominent. As a consequence of the larger coupling to the environment we expect that more decoherence is dynamically generated as the system evolves in time. The implication is that during the same time interval the distribution for $\kappa = 0.6$ evolves more rapidly to a state where much of the inference has become washed out (recall that decoherence destroys the superposition responsible for interference). This explain the lack of intermediate structure between the two distinct domains, compared to the two previous cases. Lastly, we again see that the distribution is rotated compared to the $\kappa = 0$.

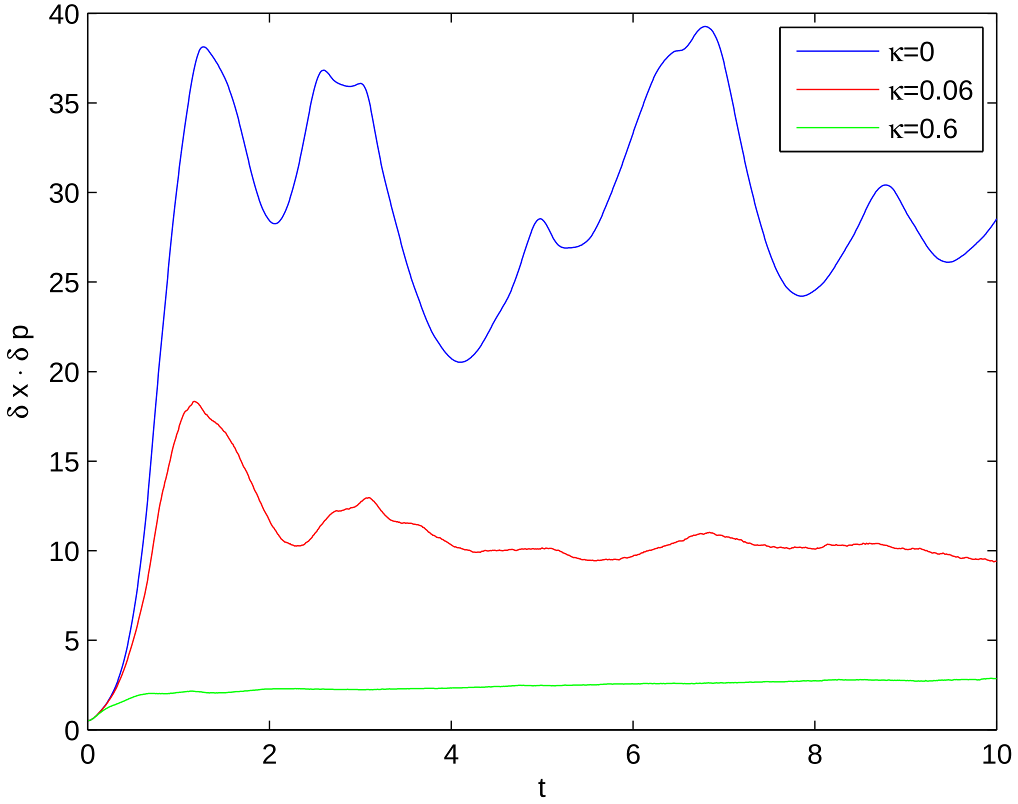

Figure 6: The width of the bosonic part of the distribution in x-p phase space as a function of time for three different coupling strengths. The system specific parameters are the same as in figure 3. As a measurement of the width of the distribution we calculate the product of the variance for x and p. The variance is defined in the usual way as $\delta x = \sqrt{\langle x \rangle^2 - \langle x^2 \rangle}$ [10] and similar for p. During the initial time-evolution the width of distribution increase to a maximum value. When the width stops to increase and begin fluctuate around a constant value we say that the system has thermalized. We note that thermalization does not necessary occur quicker nor slower when a coupling to an environment is present. The long time behaviour of the time-evolution depends on the size of phase space and thus, the photon truncation employed for the numerical simulation. This do not affect the initial results however.

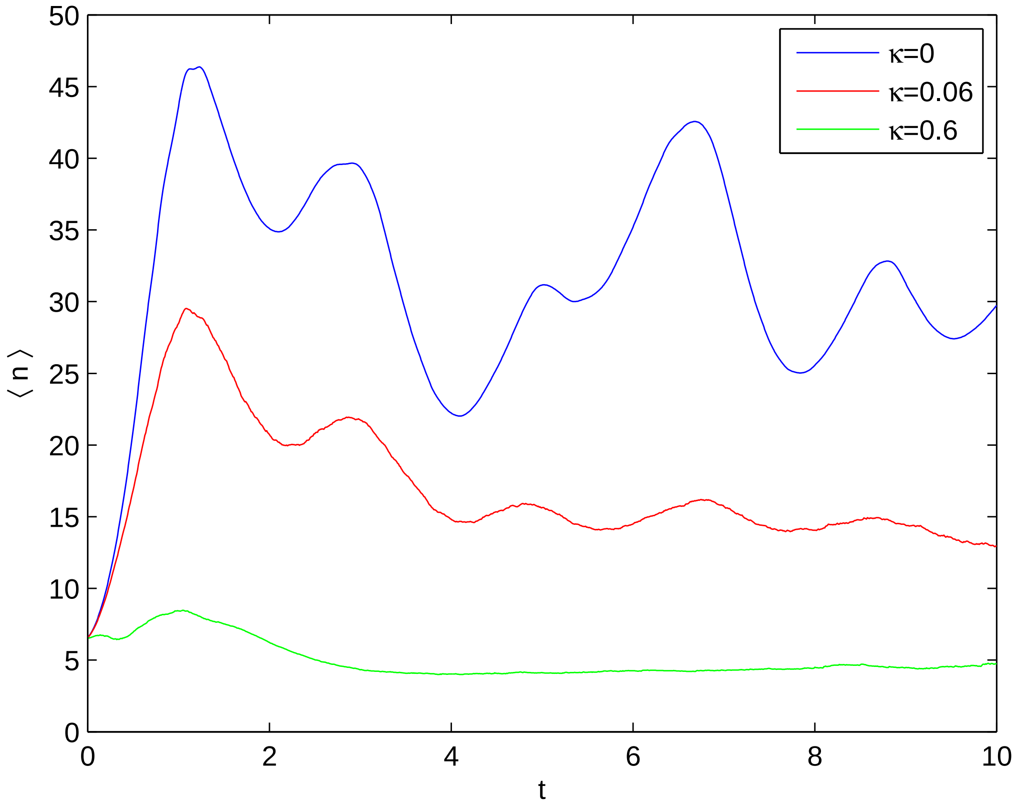

Figure 7: The expectation value of the number of photons in the system as a function of time for three different coupling strengths. The system specific parameters are the same as in figure (3). As the system-bath coupling strength is increased we see that a smaller amount of photons is present in the system. For the case $\kappa = 0.6$ we see how the system approaches equilibrium with respect to the expectation value of photons. This may seem counter-intuitive at first that not all the photons escape the system. What hinders this is the coupling of the photon field with the atoms, and the fact that excitations of the atoms create “new” photons as they become de-excited [61].

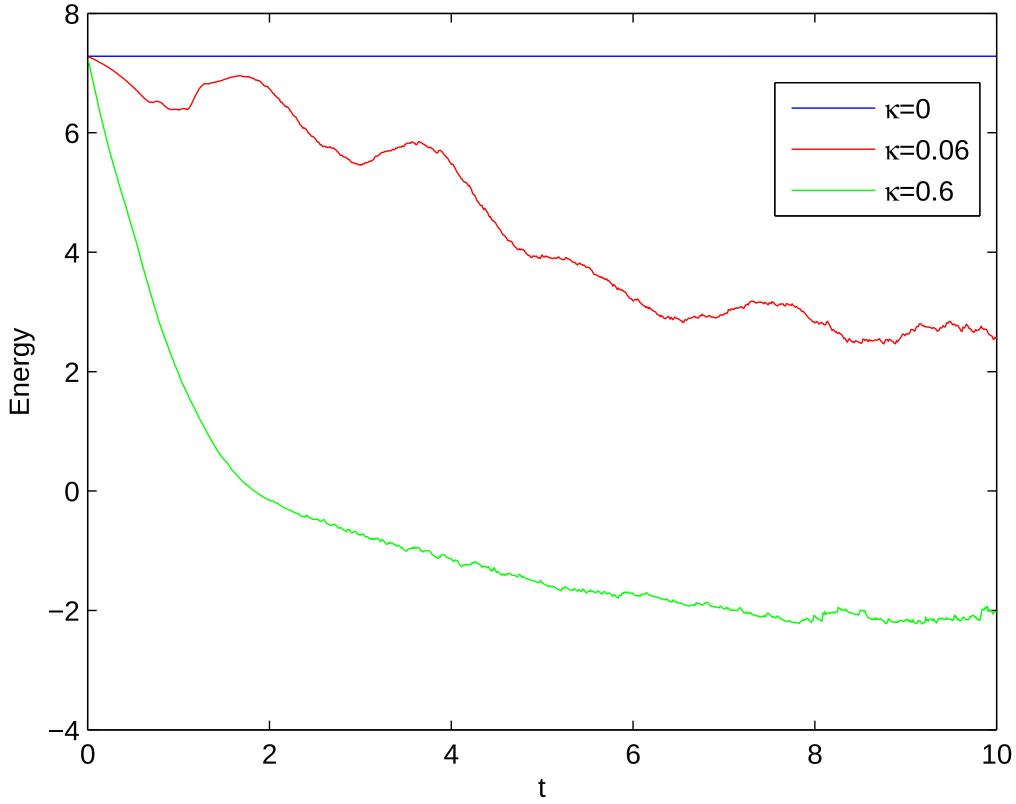

Figure 8: The energy of the system as a function of time for three different coupling strengths. As for the previous figures, the system specific parameters are the same as in figure 3. For the case when $\kappa = 0$ we have a closed system and thus the energy is a constant of the motion. When $\kappa \neq 0$ the energy is no longer conserved and decreases as the system evolves in time and lose photons to the environment.

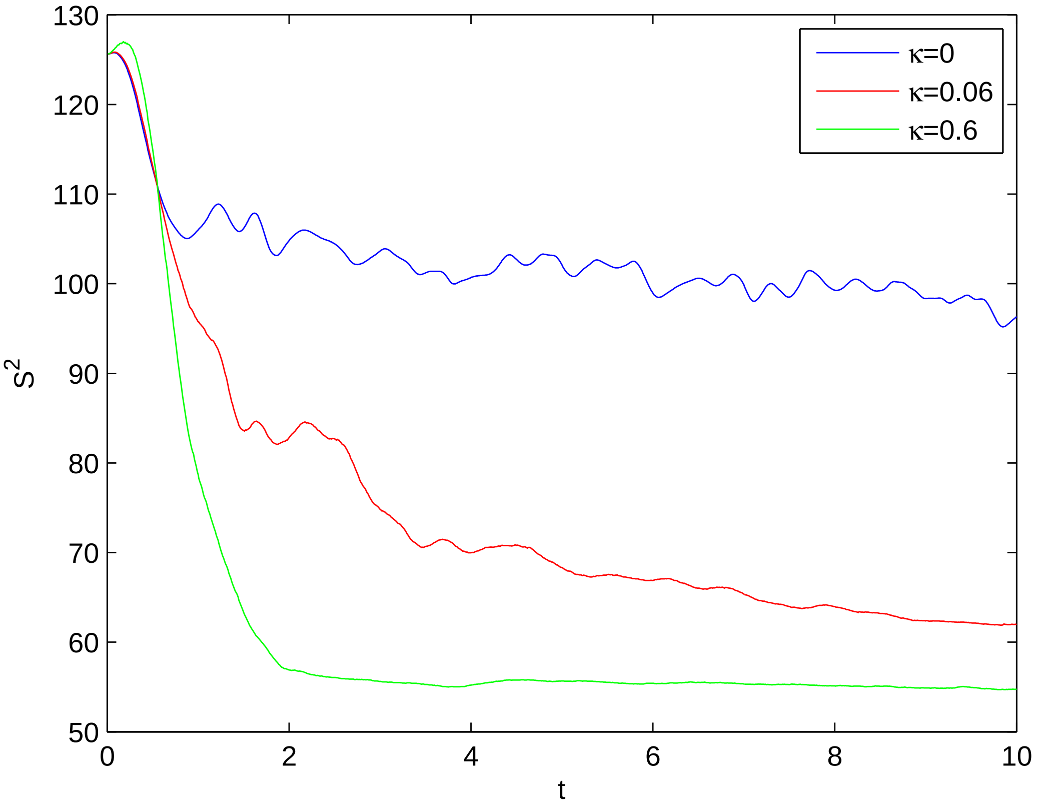

Figure 9: The square of the total spin (for the atoms) as a function of time for three different coupling strengths. The system specific parameters are the same as in figure (3). For a closed system with no interaction between its parts we expect the total angular momentum to be conserved amongst each of its parts. If, however, the system consists of different parts which interact then these parts will be entangled and we have to examine the total system to find that the spin is conserved. Hence, the examination of the spin for a subsystem of our total system can given an indication of the amount of entanglement between system parts. If we consider an open system, entanglement will also be established with the environment. The fraction of entanglement between the subsystem and the environment cannot be determined solely from the amplitude of the total spin. For a system which has thermalize we expect maximal entanglement between system parts. Note that for a short period all three cases display almost identical evolution. This time period is known as the *dwell time* [65] during which the system in some sense does not "feel" the presence of the environment.

8.2 Measuring-bath

Beyond a photon-bath we can also examine the case when the environment acts as a "measuring device" [26]. We modify our equation of motion by considering Lindblad operators that either are x or p. As a consequence, some small aspects of the quantum jump method must be modified. When the jump takes place we act with the corresponding operator we are considering. But to determine if a jump should take place or not we compare the randomly generated number with the variance of the given operator.

The idea of this section is to explore whether gaining information about either x or p will imply loss of knowledge about the conjugate variable in accordance with the Heisenberg principle. For example, if we measure x we expect that the relative width dp/dx should increase. Such an assumption is further motivated by noting that the corresponding Fokker-Planck equation for the Husimi distribution would contain a term describing diffusion in p [65]. The opposite holds true when p is measured instead. In figure 10 the numerical results are presented for the relative width. In the case of a closed system dp/dx is larger than unity once the system has thermalized. This is understood from the fact that it is x coupled to the spin in the Dicke model. When the coupling to the bath has been turned on we indeed see the localization/delocalization effect of the conjugate variables x and p.

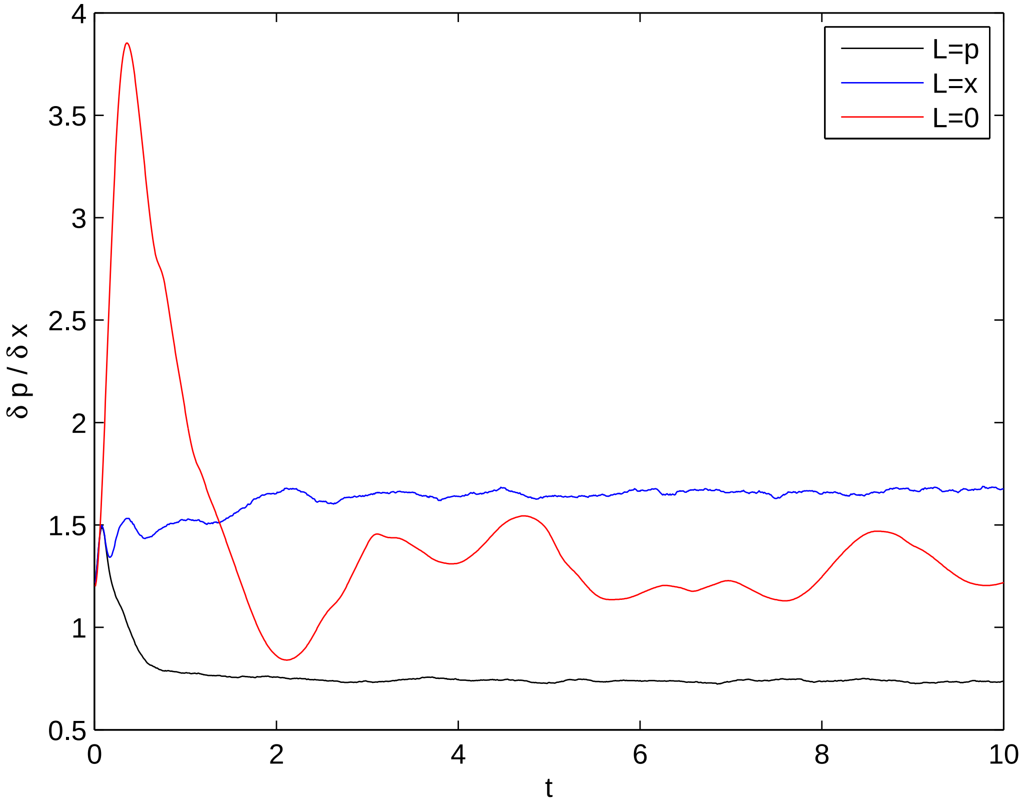

Figure 10: The ratio of the variance for p and x depending on the type of the Lindblad operator acting on the system, as a function of time. The system specific parameters are the same as in figure 3. $\kappa = 5$ is the strength of the environment-system coupling. Note that it is much larger than in previous examples. This is to clearly visualize the effect. For the case $L = x$ we have that the distribution becomes larger in the p-direction. This is in accordance with Heisenberg's uncertainty principle. Conversely, we have that the action of $L = p$ makes the distribution in the p-direction more narrow. For ergodic behaviour we expect that the long time nature of the process is to settle down. In other words, when the ration no longer changes and only fluctuation around a fixed value take place. The implication of this is that the system has thermelized with respect to the "measuring" environment. Within the marginal of errors (fluctuations due to other sources) it appearers, as in the previous case, that the closed system and the open ones thermalize roughly at the same time.

9 Conclusion and Summary

In this thesis we have examined how quantum thermalization is affected when the system in question is connected to an environment. Working with the assumption that chaos and thermalization are related, an idea borrowed from classical mechanics, we proceeded to pick a system characterised by the Dicke Hamiltonian. It is known that as an isolated system, the Dicke Hamiltonian exhibits signatures of quantum chaos manifested by for example the distribution of energy-level spacing. Coupling this system to an environment, one would imagine that thermalization would be reached faster. For a classical open system this is something that is well known from everyday experience, and as well as from statistical mechanics. Even from a quantum mechanical viewpoint we expect this to be true. An isolated system will evolve in time in a unitary fashion which is well known from fundamental quantum theory. This means that an initially given pure state describing the system will remain pure for all times. This is in direct contrast to a thermal state which is not pure. Why this is the case can easily be realised if we think about a classical analogy. Considering an isolated system, for example an empty room at some set temperature. If we were to open a hatched and throw in a hot plate, only for then to immediately close it again, the system would again be isolated. After some time the isolated system will have distributed this disturbance temperature uniformly throughout the system. Quantum mechanically this would imply that the system state is non-pure as it contains information about every part of the system. In other words, every part of the system is entangled amongst its parts. Yet, for a classical system it is possible for thermalization to take place in an isolated system, where for a quantum mechanical one it seems that this is impossible. However, experimentally it is established that even isolated quantum systems do thermlize. To explain this fact quantum chaos is often invoked as an explanation. As a consequence of the repelling of energy-levels related to chaotic behaviour, the system will posses a large number of time-scales on which it evolves. Forming the total system state as the superposition of these states causes in the long time limit destructive inference. The result of this is a time-independent final state which has reached equilibrium. This is the most common theoretical explanation to why isolated quantum systems can reach thermal equilibrium (or to be exact steady-state). It is satisfying that chaos is the cause for thermalization in both the classical and quantum world. Returning to the issue of an open system we have that the system no longer have to evolve by unitary time-evolution. The implication follows directly; an initially pure state no longer have to remain pure. It is this assertion that is the root of the assumption that an isolated quantum system which is known to thermalize, should do so at a quicker rate when connected to an environment.

With this in mind we proceed to discuss the required theoretical tools needed to study this scenario. Beyond the obvious inclusion of theory concerning open systems and chaos, we also focused on the fundamentals of quantum theory expressed in the often overlooked phase space formulation of quantum mechanics. It is in this framework that quantum chaos expresses itself most clearly. During the course of this establishment of theory, a crucial realisation can be made, thermalization is not the only effect which should be aided by the connection to an environment. Decoherence, an effect which is known to destroy quantum behaviour such as the important concept of superposition, is known to set in for quantum system in contact with an outside source. It is by decoherence a quantum system can evolve to a classical system obeying our everyday experience. Studying the combination of these two naturally expected effects was a main goal of this thesis. As was discussed in chapter 5 these two effects seems to be contradicting when it comes to predictions of the rough behaviour of the system, characterised by the phase space formulation as a distribution. Realising this staggering contradiction we set out to examine this set-up in more detail to determine which effect would reign supreme and how the time-evolution of the system would be affected.

With the knowledge of an open quantum system we determined that the time-evolution of the system can be given by a master equation. Solving this by utilising an approximate method known as the quantum jump method we obtained the density matrix for the system. From this we used our know how of phase space quantum mechanics to transform it to into a phase space quasi-distribution. Examining this distribution guided us to identify ergodicity, a hallmark feature of classical chaos theory, for the closed system. Letting the coupling to the environment be non-zero, we proceed to the uncharted intersection of decoherence and thermalization caused by the mentioned environment.

In chapter 8 we presented the results related to our problem set-up. We found that a connection with an environment caused an initially localised distribution to remain localised for longer. This is in contrast to what one would expect when it comes to thermalization which rest on the fact that the distribution spreads out ergodically in phase space. Yet, it is exactly what we would expect as a consequence of decoherence. Here it is also interesting to go back to the equation of motion for the Husimi distribution given in Eq.(6.17). As already mentioned, the presence of the bath enters for example in a diffusion term, which naively suggests that the spreading should be occurring faster. The results, however, shows the opposite showing that the spreading in quantum systems is at least partly driven by interferences within the quantum state. Further indications that the phase space distribution thermalized roughly at the same time regardless of an connection to an environment were found when the width in x and p was plotted in figure 6. We found that the point of constant width occurred approximately at the same time. The implication from this is that the system thermalizes (reaches steady state) more or less at the same time. Changing the environment from a photon-bath to a measuring inducing surrounding we proceeded to again examining the width of the distribution (or more exact the ration of the x- and p-widths). The results obtained pointed in the same direction as the one for the photon-bath. We once more saw that thermalization occurred around the same time. An attempt to try and explain this phenomena could focus on relevant time-scales for the system compared to the environment induced coupling. If thermalization truly occurs at the same time regardless of connection to an environment then it would imply that time-scales on which thermalzation takes place is determined primarily by the isolated system. This means that thermalzation is foremost an effect of isolated quantum systems, and not of open ones. Still, it must be so that a sufficiently large coupling strength to an environment at some point overpowers the system time-scale[46]. Realising this could provided insight to the microscopic origins of the laws of thermodynamics. Moreover, this result can also be taken as an indication on the nature of quantum chaos. It is a not too uncommon opinion amongst non-specialist that by definition (unitary time-evolution) chaos cannot take place in isolated quantum systems [32]. But if thermalization is determined primarily by the dynamics of the isolated system and not the connection to the environment then that means that the dynamic generated in the isolated system is sufficient to cause the offset of chaos. Hence, an isolated system that thermalizes indicates that chaos indeed do exist in quantum mechanics (and can develop in isolated quantum systems).

No conclusion would be complete without a discussion on how reliable these results are. To start with, it is important to keep in mind that these results are system specific. There exist no guarantee that the same indications can be found for other system and environment configurations. Still, many times system specific studies gives an indication of possible general behaviour for a large class of systems. A factor which we have failed to mention up to this point is the following, which can greatly affect the obtained results. When a connection to a photon-bath is established the available phase space shrinks due to dissipation of photons. This is easy to understand as the possible number of configurations for the system decrease. The fact that the available phase space volume is different depending on the connection with the environment makes the analysis of the results more difficult. This is especially true when we examine ergodicity. In principle this could be bypassed by examining other quantities, but some trace of this problem could very well still be present.

There exist a last variety of topics which can be studied in the future which build

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[46] When deriving the master equation we do it by imposing a number of approximations. One of them being that the coupling of the system and environment is not too large.

upon or are related to what we have done here. The most direct continuation would be to examine the spin part of the quasi-probability distribution in order to determine how it is affected by the system-environment coupling. Naturally, it would be desirable to also qualitatively measure how the thermalization time depends on the coupling strength of κ. For example, when does the weak κ dependence break down, and for regular systems (non-chaotic) we should not have this weak coupling dependence so could one actually use this as an indicator of chaos? In addition, we could investigate other properties related to thermalization. One example is expectation values which for a system which has thermalized should be time-independent. Another possibility would be to considerer a different system and/or environment to examine if these results appears to be universal. We can employ largely the same methods to study these different configurations. Prime candidate to examine would be systems were the quantum version is chaotic, while the classical one is not. Regardless of what road is chosen for future studies one thing is clear, the quest to fully understand quantum thermalization, integrability and chaos will continue.

A Appendix

In this chapter we present necessary theory specific to the system under consideration in this thesis, or methods used to obtain the results presented in chapter 8.

A.1 The Dicke Hamiltonian

In this appendix we will derive the general form of the Dicke Hamiltonian which is our starting point for the result section in this thesis. We will omit any special indication on what quantities which are operators, it should be apparent from context when we are dealing with operators or not. This form of the Hamiltonian appears when examining how light interact with matter on a quantum level. Hence, we consider the case of a system consisting of an atom with a single electron with charge e and mass m constrained by the potential $V(\mathbf{x})$, and a electromagnetic field characterised by the vector potential $\mathbf{A}(\mathbf{x}, t)$. The Hamiltonian describing this atom-field interaction can be formulated by using the minimal substitution procedure [15] yielding

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{e\mathbf{A}}{c}\right)^2 + V(\mathbf{x}) + H_F = H_A + H_F + H_I \tag{A.1}$$

with H_F the free Hamiltonian belonging to the quantized electromagnetic field[47] [24]

$$H_F = \sum_{kj} \hbar \omega_k a^\dagger_{kj} a_{kj}, \tag{A.2}$$

the free Hamiltonian representing the atom

$$H_A = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \tag{A.3}$$

with $\mathbf{x}$ the relative position of the electron from the nucleus and $\mathbf{p}$ corresponding to the momentum for the electron; lastly we defined the interaction part of the Hamiltonian between the atom and field as

$$H_I = -\frac{e}{2mc}(\mathbf{p}\ \mathbf{A} + \mathbf{A}\ \mathbf{p}) + \frac{1}{2m}\left(\frac{e\mathbf{A}}{c}\right)^2. \tag{A.4}$$

The term containing the square in Eq.(A.4) is small compared to the first term as it contains the electric charge e^2. In addition, it is known from quantum field theory [24] and the mode expansion of the vector potential, that the second term in Eq.(A.4) represent the interaction between different modes of the electromagnetic field coupled via the present electron. In other words, the process described by the second term corresponds to a two-photon transition process which we will disregard as a consequence of its smallness (the amplitude for these processes are small). With this Eq.(A.4) can be approximated by

$$H_I \approx -\frac{e}{2mc}(\mathbf{p}\ \mathbf{A} + \mathbf{A}\ \mathbf{p}) = -\frac{e}{2mc}\left[\mathbf{A}, \mathbf{p}\right]_+. \tag{A.5}$$

The mode expansion of $\mathbf{A}(\mathbf{x}, t)$ is given by [24]

$$\mathbf{A}(\mathbf{x}, t) = \sum_{kj} \lambda_{kj} \left(a_{kj} e^{-i\mathbf{k}\ \mathbf{x}} + a^\dagger_{kj} e^{i\mathbf{k}\ \mathbf{x}}\right) \tag{A.6}$$

with $\mathbf{k}$ the wave vector, a and $a^\dagger$ destruction and creation operators for oscillations in the field (in order words photons), the sum over k with respect to different modes (associated with different wave vectors), and the sum over j referring to the various polarisation modes occurring in for example the definition of λ_{kj}

$$\lambda_{kj} = \sqrt{\frac{2\pi\hbar c^2}{V\omega_k}}\mathbf{e}_{kj}. \tag{A.7}$$

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[47] We will not use the full covariant formulation of the electromagnetic field as the situation does not call for relativistic considerations.

where $\mathbf{e}_{kj}$ are real unitary orthogonal vectors, V is the volume of the area ("box") where the field is contained, and ω_k is the frequency. From Eq.(A.6) it is apparent that $\mathbf{A}(\mathbf{x},t)$ and $\mathbf{p}$ do not commute. If we however invoke the dipole approximation [66] we can solve this grievance. Considering in more detail the typical atomic range which is approximately given by the Bohr radius $5.3 \cdot 10^{-11}m$ and the wavelength of visible light $10^{-6}m$. With these values we have that $k = \frac{2\pi}{\lambda} \approx 2\pi \cdot 10^{-6}m^{-1}$ and therefore $\mathbf{k} \cdot \mathbf{x} \approx 3.5 \cdot 10^{-4} \ll 1$ and as a consequence $e^{i\mathbf{kx}} \approx e^0 = 1$, resulting in $\mathbf{A}(\mathbf{x}) \approx \mathbf{A}(0)$. By performing this approximation we are in fact ignore the effect of the position of the electron when examining the interaction between the field and the atom. With this the commutator between $\mathbf{A}$ and $\mathbf{p}$ is now equal to zero, and the anti-commutator in Eq.(A.5) becomes two times the product. That way

$$H_I = -\frac{e}{mc}\mathbf{A}(0)\mathbf{p}. \tag{A.8}$$

This expression can be further refined by relating the electron momentum operator p to the atomic pseudo-spin operators. Recalling that the Hamiltonian can be represented as

$$H_A = \sum_n E_n \left|n\right\rangle \left\langle n\right| \tag{A.9}$$

where E_n is the eigenvalue of H_A and $\left|n\right\rangle$ the corresponding eigenvectors. This representation can be generalised by introducing a group of generalised atomic operators

$$\sigma_{nm} = \left|n\right\rangle \left\langle m\right|, \tag{A.10}$$

then we can write H_A as

$$H_A = \sum_n E_n \sigma_{nn}. \tag{A.11}$$

By considering this as a base in the associated Hilbert space belonging to the atom we can express any (atom related) operator as

$$G = \sum_{n,m} \left\langle n\right| G \left|m\right\rangle \sigma_{nm}. \tag{A.12}$$

From Eq.(A.10) it follows that the atomic operators satisfy the commutation relation

$$[\sigma_{ij}, \sigma_{kl}] = \delta_{jk}\delta_{il} - \delta_{il}\delta_{kj}. \tag{A.13}$$

For the case of a two-level atom[48] the atomic operators can be explicitly determined as there is only two possible energy eigenstates, the lower $\left|-\right\rangle$ and the higher $\left|+\right\rangle$. Hence

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[48] In such a *two-level approximation* we assume that only two electronic states of the atom are of importance, e.g. any other transitions between electronic states are far detuned from the field frequencies such that they can be neglected.

$$\sigma_{11} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_{12} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad \sigma_{21} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \sigma_{22} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}.$$

With this we can construct the pseudo-spin operators

$$S_z = \frac{1}{2}(\sigma_{22} - \sigma_{11}), \quad S_+ = \sigma_{21}, \quad S_- = \sigma_{12} \tag{A.14}$$

which satisfy the standard commutation relations

$$[S_z, S_\pm] = \pm S_\pm, \quad [S_+, S_-] = 2S_z, \quad [S_+, S_-]_+ = \mathbb{1}, \tag{A.15}$$

as can be checked by using Eq.(A.13). The name spin operators can be a bit misleading as it is not a spin in the traditional sense we are referring to here. What we are referring to is the two possible energy-states (electronic Zeeman levels) the atom can be in. This is akin to a spin 1/2 particle which can be either in the state "pointing" down or up in any preferred direction. As a consequence of this similarity we have an identical algebra for these cases. Hence the name pseudo-spin operators. Writing the momentum operator $\mathbf{p}$ using Eq.(A.12) we have[49]

$$\mathbf{p} = \langle +|\,\mathbf{p}\,|-\rangle\, S_+ + \langle -|\,\mathbf{p}\,|+\rangle\, S_-. \tag{A.16}$$

To evaluate these terms we note

$$\frac{d}{dt}\mathbf{x} = \frac{1}{i\hbar}[\mathbf{x}, H_A] = \frac{\mathbf{p}}{m}, \tag{A.17}$$

which is a general result for a Hamiltonian on the form as in Eq.(A.3). Using this and the eigenvalue equation for the free Hamiltonian $H_A\,|n\rangle = E_n\,|n\rangle$, we obtain for each term

$$\langle +|\,\mathbf{p}\,|-\rangle = \frac{im}{\hbar}(E_+ - E_-)\,\langle +|\,\mathbf{x}\,|-\rangle = \frac{im\omega_0}{\hbar e}\,\langle +|\,e\mathbf{x}\,|-\rangle \tag{A.18}$$

and

$$\langle -|\,\mathbf{p}\,|+\rangle = -\frac{im\omega_0}{\hbar e}\,\langle -|\,e\mathbf{x}\,|+\rangle\,, \tag{A.19}$$

where we have denoted $E_+ - E_- = \hbar\omega_0$ for the energy difference. We can proceed by identifying that $\langle +|\,ex\,|-\rangle$ is the matrix element of the atomic dipole operator $e\mathbf{x}$, meaning that it is natural to introduce the dipole operator $\mathbf{D}$,

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[49] In principle diagonal elements could also be included. These would, however, give a zero contribution (as they are odd).

$$\langle + |\, e\mathbf{x}\, | - \rangle = i\mathbf{D} \tag{A.20}$$

where $\mathbf{D}$ is a real vector. With this we can express the momentum operator using the pseudo-spin operators and the real vector $\mathbf{D}$ as

$$\mathbf{p} = -\frac{m\omega_0}{e}\mathbf{D}(S_+ + S_-). \tag{A.21}$$

With this and the expression for $A(0)$ (which follows from Eq.(A.6) setting the exponentials to one) we have for the interaction Hamiltonian

$$H_I = -\frac{e}{mc}\sum_k (a_k^\dagger + a_k)\lambda_k \left(-\frac{m\omega_0 \mathbf{D}}{e}\right)(S_+ + S_-) = \sum_k \epsilon_k (a_k^\dagger + a_k)(S_+ + S_-) \tag{A.22}$$

where we defined the atom-field coupling constant as

$$\epsilon_k = \sqrt{\frac{2\pi\hbar}{V\omega_k}}\omega_0 \mathbf{D}\cdot\mathbf{e}_{kj} \qquad (j = 1, 2) \tag{A.23}$$

and where we have dropped the sum over j by assuming that one of the polarisation axes is parallel to the dipole operator $\mathbf{D}$. Employing the pseudo-spin operators we can also eliminate the presence of $\mathbf{p}$ in the free Hamiltonian

$$H_A = E_+\sigma_{22} + E_-\sigma_{11} = \frac{\hbar\omega_0}{2}(\sigma_{22} - \sigma_{11}) = \hbar\omega_0 S_z \tag{A.24}$$

provided that we choose $E_+ + E_- = 0$.

Collecting all parts we have for the total Hamiltonian

$$H = \sum_k \hbar\omega_k a_k^\dagger a_k + \hbar\omega_0 S_z + \sum_k \epsilon_k (a_k^\dagger + a_k)(S_+ + S_-), \tag{A.25}$$

which is known as the *multi-mode Rabi model Hamiltonian.* The first two parts corresponds to the energy contained in the electromagnetic field as measured by the amount of photons in different modes (first term); and the energy associated with which energy level is populated in the atom which is related to the z component of the pseudo-spin operator (the second part). The third term deserves a closer look, for clarity we write it as

$$H_I = \sum_k (a_k^\dagger S_- + a_k S_+ + a_k^\dagger S_+ + a_k S_-). \tag{A.26}$$

The analysis of the interaction part is straightforward in this form. The first term represent the process where an atom in the higher state transit down to the lower and emit a photon, the opposite is true for the second term where the atom absorbs one photon and then gets excited from the lower to the higher state. For the remaining terms we have the seemingly odd situation of excitation and the creation of a photon (the third term), and de-excitation and the absorption of a photon (the forth term). One way to examine the validity of each of these processes is to check energy conservation. Defining the energy difference between the associated atom state and the photon as

$$\Delta E_1 = \hbar(\omega_k - \omega_0). \tag{A.27}$$

For energy conservation to hold $\Delta E \approx 0$ we must have $\omega_k \approx \omega_0$ (resonant case). If this is the case then the energy-time uncertainty relation

$$\Delta E_1 \Delta \tau_1 \geq \hbar \tag{A.28}$$

tells us that as $\Delta E_1 \to 0$, then $\Delta \tau_1 \to \infty$. The implication of this is that the accredited photons have a long life time and can thus be identified as real photons. This is the case for the first two terms. For the third and fourth term we have instead the energy difference

$$\Delta E_2 = \hbar(\omega_k + \omega_0), \tag{A.29}$$

this expression prohibits the conservation of energy, and as such these situations can not produce any real photons. We see this again from considering the energy-time uncertainty relation

$$\Delta E_2 \Delta \tau_2 \geq \hbar \tag{A.30}$$

and noting that the implication from the non-zero size of ΔE_2 (and that is value is large) is that $\Delta \tau_2$ must be very small. Hence, the photons occurring in the last two terms are virtual photons with a very short life time. Excluding these terms which temporally violate energy conservation, known as the *rotating wave approximation*[50], allows us to write the Hamiltonian on the form

$$H_{RWA} = \sum_k \hbar\omega_k a_k^\dagger a_k + \hbar\omega_0 S_z + \sum_k \epsilon_k (a_k^\dagger S_- + a_k S_+). \tag{A.31}$$

which is known as the *multi-mode Rabi Hamiltonian in the rotating wave approximation* [66, 67]. In the very strong coupling regime (the atom-light coupling is comparable to the frequencies ω_k and ω_0) this approximation breaks down and we must include all four terms of Eq.(A.26). This is far reaching consequences since the model with or without the rotating wave approximation is either integrable or non-integrable. For

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[50] See [15] for a more precise discussion. The argument made here can be supplemented with more exact mathematical statements.

chaos to set in we must be in the very strong coupling regime. The result is that we will not impose the rotating wave approximation.

The procedure in this derivation can be generalised to an N-atoms system by introducing the collective pseudo-spin operators [67]

$$S_{\pm} = \sum_{i=1}^{N} S_{\pm}^{(i)}, \quad S_z = \sum_{i=1}^{N} S_z^{(i)}, \tag{A.32}$$

as well as restricted to just one mode of the radiation field[51] by not summing over k (i.e. considering a fixed value of k). When doing this we obtain the *Dicke Hamiltonian.* The dissimilarity between Dicke and the Rabi model is that we consider many particles in the Dicke model, otherwise they are similar.

The Dicke Hamiltonian exhibits a number of interesting properties which are discussed in [67]. Among the most interesting ones is the occurrence of a phase transition in the thermodynamic limit which for the Dicke model implies letting the spin (number of particles) go to infinity; and of course the presence of quantum chaos.

A.2 The Quantum Jump/ Monte Carlo wave-function method

In this appendix we will outline the *quantum jump* (also known as *Monte Carlo wave-function*) method. We will closely follow the arguments laid out in [68]. The quantum jump method will be used to numerically calculate the time-evolution of the density matrix. The validity of this method rest on the fact that it can be shown to be equivalent with the master equation formulation.

From chapter 3 we know that a general (Born-Marakov) master equation can be formulated as

$$\dot{\rho}_S = \frac{i}{\hbar}\left[\rho_S, H_S\right] + \mathcal{L}_{relax}(\rho_S), \tag{A.33}$$

with $\mathcal{L}_{relax}$ the relaxation superoperator related to the connection of the system S with an environment (compare with Eq.(3.31)). The form of relaxation operator explicitly under consideration here is

$$\mathcal{L}_{relax}(\rho_S) = -\frac{1}{2}\sum_m \left(L_m^{\dagger} L_m \rho_S + \rho_S L_m^{\dagger} L_m\right) + \sum_m L_m \rho_S L_m^{\dagger}. \tag{A.34}$$

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[51] Considering just a single mode is justified since we have in mind a set of atoms confined within a cavity/resonator with discrete photon modes and only one of them is resonant (or quasi-resonant) with the corresponding atomic transition.

The L_m operators act in the state space of the sub-system S and can for example in the case of a harmonic oscillator be taken to be

$$L^\dagger = a^\dagger, \quad L = a, \tag{A.35}$$

this would correspond to a bosonic system where there is only one operator in the sum over m. With the definitions out of the way we proceed to state the procedure for time-evolving the sub-system wave function $|\phi(t)\rangle$ to a later time $t + \delta t$. This can be summarised into three steps:

1. First we calculate the infinitesimal time-evolution of $|\phi(t)\rangle$ with a non-Hermitian Hamiltonian as the generator

   $$H = H_S - \frac{i\hbar}{2} \sum_m L_m^\dagger L_m, \tag{A.36}$$

   giving

   $$\left|\phi^{(1)}(t+\delta t)\right\rangle = \left(1 - \frac{iH\delta t}{\hbar}\right) |\phi(t)\rangle . \tag{A.37}$$

   As the Hamiltonian H is non-Hermitian the time-evolution does not preserve the norm, i.e. it is not unitary. In order to preserve the norm of the state we calculate the square of the norm (ignoring terms of second order in δt)

   $$\begin{aligned} &\left\langle\phi^{(1)}(t+\delta t)\right| \left|\phi^{(1)}(t+\delta t)\right\rangle = \\ \langle\phi(t)| \left(1 + \frac{iH^\dagger \delta t}{\hbar}\right)\left(1 - \frac{iH\delta t}{\hbar}\right)|\phi(t)\rangle = 1 - \delta t \frac{i}{\hbar} \langle\phi(t)|\, H - H^\dagger \,|\phi(t)\rangle &= \\ 1 - \sum_m \delta t \,\langle\phi(t)|\, L_m^\dagger L_m \,|\phi(t)\rangle . \end{aligned} \tag{A.38}$$

   The sum over m in the last line of the above equation $\delta p = \sum_m \delta t \,\langle\phi(t)|\, L_m^\dagger L_m \,|\phi(t)\rangle$ can be seen to always be greater then or equal to zero (otherwise the norm could be larger then one!)[52]. If the time-evolution is to be infinitesimal we must also have that $\delta p \ll 1$, which can be made possible by choosing small time steps δt.

2. The second step is that which constitute the "quantum jump". When the wave function evolves from t to $t + \delta t$ we introduce the possibility for a quantum jump,

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[52] This also follows from the fact that the norm of $L_m|\phi(t)\rangle$ is contained in the sum, which is always positive.

related to the stochastic nature of an open quantum system. To determine if a jump takes place between t and $t + \delta t$ we pick a random number ϵ in the interval 0 to 1 and then compare it to δp. For the case $\delta p < \epsilon$ no quantum jump takes place and we write the propagated normalised wave function as

$$|\phi(t+\delta t)\rangle = \frac{1}{\sqrt{(1-\delta p)}} \left|\phi^{(1)}(t+\delta t)\right\rangle . \tag{A.39}$$

This will most often be the case because $\delta p \ll 1$. If we have the other possibility, namely that $\epsilon < \delta p$, then a quantum jump will occur. This jump will affect the wave function in such a way that we pick $L_m |\phi(t)\rangle$ as the propagated wave function. Which of the operators m that are chosen are determined according to the probability relation

$$P_m = \frac{\delta t \langle\phi(t)| L_m^\dagger L_m |\phi(t)\rangle}{\delta p}, \tag{A.40}$$

if we are dealing with a system where only one operator L_m is present then $P_m = 1$. The normalised propagated wave function, after a quantum jump has taken place, is written as

$$|\phi(t+\delta t)\rangle = \frac{1}{\sqrt{\langle\phi(t)| L_m^\dagger L_m |\phi(t)\rangle}} L_m |\phi(t)\rangle , \tag{A.41}$$

here we do not use the same normalisation factor as for the other case, no infinitesimal time-evolution has taken place in the traditional sense.

3. In order to get a correspondence (which we will see in the next section) with the master equation formulation we have to repeat this process a number of times and take the average (it is in this sense we talk about a Monte Carlo wave function method). With this we can form the density operator in the usual way $\rho(t) = \overline{\left|\phi(t)\right\rangle \left\langle\phi(t)\right|}$.

For this method to carry any validity it must be equal to the time-evolution master equation that we postulated that ρ must obey. Defining $\sigma(t) = |\phi(t)\rangle\langle\phi(t)|$ we want the average of this quantity, $\overline{\sigma}$, to be equal to $\rho_S(t)$ provided that they are the same at time $t = 0$. Following this we examine the average of $\sigma(t + \delta t)$ with respect to the time-evolution, which is given by

$$\begin{aligned} \overline{\sigma(t+\delta t)} = (1-\delta p) \frac{1}{\sqrt{1-\delta p}} |\phi(t+\delta t)\rangle \frac{1}{\sqrt{1-\delta p}} \langle\phi(t+\delta t)| + \\ \delta p \sum_m P_m \frac{1}{\sqrt{\langle\phi(t)| L_m^\dagger L_m |\phi(t)\rangle}} L_m |\phi(t)\rangle \frac{1}{\sqrt{\langle\phi(t)| L_m^\dagger L_m |\phi(t)\rangle}} \langle\phi(t)| L_m^\dagger, \end{aligned} \tag{A.42}$$

with the first part corresponding to the no-jump process and the second to the case where a quantum jump occurs. Employing Eq.(A.37) and again disregarding quadratic terms in δt we get

$$\begin{aligned}\overline{\sigma(t+\delta t)} = \left|\phi(t)\right\rangle \left\langle\phi(t)\right| + \frac{iH\delta t}{\hbar}\left|\phi(t)\right\rangle \left\langle\phi(t)\right| + \left|\phi(t)\right\rangle \left\langle\phi(t)\right| \frac{iH^{\dagger}\delta t}{\hbar} + \\ \delta p \sum_{m} P_m \frac{1}{\left\langle\phi(t)\right| L_m^{\dagger} L_m \left|\phi(t)\right\rangle} L_m \left|\phi(t)\right\rangle \left\langle\phi(t)\right| L_m^{\dagger}.\end{aligned} \tag{A.43}$$

Using the definition of the total non-Hermitian Hamiltonian given in Eq.(A.36), along with the definition of δp, we arrive at

$$\overline{\sigma(t+\delta t)} = \sigma(t) + \frac{i\delta t}{\hbar}\left[\sigma(t), H_S\right] + \delta t \mathcal{L}_{relax}[\sigma(t)]. \tag{A.44}$$

If we now average this expression over all possible values of $\sigma(t)$ and take the time limit $\delta t \to 0$ we obtain

$$\dot{\overline{\sigma}} = \frac{i}{\hbar}\left[\overline{\sigma}, H_S\right] + \mathcal{L}_{relax}[\overline{\sigma}] \tag{A.45}$$

which is on the exact same form as the master equation given in Eq.(A.33). Thus, we have shown that the quantum jump method of calculating the time-evolution for a sub-system is equal to solving the corresponding master equation for the density matrix.

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