Bachelor thesis in physics

Criticality in an open quantum system

Julia Hannukainen

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Supervisor: Ass.prof. Jonas Larson
Department of Physics/
Condensed Matter and Quantum Optics
Stockholm University

Abstract

The theory of critical phenomena is well understood for both classical and quantum mechanical systems in equilibrium. For these systems a continuous phase transition, with specified critical exponents, is accompanied by a spontaneous symmetry breaking; where a critical point separates a phase sharing the same symmetry as the system Hamiltonian from a phase where this symmetry is broken. The theory of criticality is, however, not well established for open quantum systems, systems driven far from equilibrium. But with advancement in experimental techniques, it is now possible to create and control these types of systems, evoking an interest to ask questions about criticality and universality. In this thesis the critical behaviour of such an open quantum system is established by considering a solvable model supporting a phase transition. The results show that the phase transition is continuous and two critical exponents are given. However, in contrast to systems in equilibrium, no spontaneous symmetry breaking occurs across the critical point.

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1 Introduction

The purpose of this thesis is to explore critical phenomena of an open quantum system, a system which is coupled to an environment, i.e. a system out of equilibrium. Critical phenomena is a concept related to phase transitions, the abrupt change in the macroscopic behaviour of a system when external conditions such as pressure and temperature are varied [1]. The point where this happens is called a critical point and the corresponding phase transitions are divided into different types depending on how the system behaves in the vicinity of the critical point [1]. One such type of phase transitions is called *continuous* phase transitions, these are characterised by the fact that many of the thermodynamic quantities between the phases approach zero smoothly at the critical point, and that the correlation length, the length scale over which the particles are correlated, diverges at the critical point, so that there exists a single critical phase [1]. Continuous phase transitions are divided into *universality classes* governed by global features, such like the symmetries of the Hamiltonian of the system [1]. Microscopic details of a system turn out to be non-important when describing its behaviour close to a critical point, so many different systems, with regards to microscopic details, belong to the same universality class and are described by the same mathematical functions [1]. The different universality classes are defined by their *critical exponents*. If the behaviour of an order parameter, η can be written as a function of a system parameter λ close to a critical point λ_c as $\eta \propto |\lambda_c - \lambda|^\nu$, then the exponent ν is the critical exponent, and thus all continuous phase transitions with the same exponents fall under the same universality class [1].

The critical behaviour of systems in equilibrium, both classical and quantum mechanical are well studied and understood. The phase transition of such a system, for example a system in equilibrium at temperature $T = 0$ and with the transition driven by quantum fluctuations, is commonly accompanied by a *spontaneous symmetry breaking* [2]. This means that a phase possessing the same symmetries as the underlying Hamiltonian is transitioned into a phase where this symmetry is broken; the energy function of the system thus goes from having one stable point, to having at least two, which one of these the system chooses will depend on its previous history [2]. The critical behaviour of open quantum systems is not as well analysed nor understood. But with advancement in technology, it is now possible to control and sometimes even tailor a system after ones own need, and it is even possible to control the coupling between a system and its environment [3]. Thus, if a non-equilibrium state may be created, it is of interest to explore and get an understanding of the critical behaviour and universality (if they exist) of such systems.

A solvable model which supports a phase transition will be considered in this thesis, in order to explore criticality in an open system. The time evolution of an open system may not be carried out through a unitary transformation of the Hamiltonian, which is the method used for closed systems [4]. The approach is instead to use a quantum master equation, an equation derived by imposing certain approximations on the combined system, the system of interest together with its environment [4]. The master equation used will be of the *Lindblad form*; the system will consist of a large spin quantum number, s, where the unitary part of the evolution of the system is due the Hamiltonian consisting of the x- components, $\hat{S}_x$, of the spin operators. The coupling to the environment is taken into account through so called *jump operators*, and it is these that makes the full time evolution non-unitary. The jump operator for the model studied is the spin lowering operator, $\hat{S}_-$. The Lindblad equation describing the time evolution of the state ρ thus has the form

$$\dot{\rho} = -i\left[\omega \hat{S}_x, \rho\right] + \frac{\kappa}{s}\left(2\hat{S}_-\rho\hat{S}_+ - \hat{S}_+\hat{S}_-\rho - \rho\hat{S}_+\hat{S}_-\right), \tag{1.1}$$

where ω and κ are constants. Criticality in a Lindblad equation means non-analytic properties of the equation's steady state, i.e. ρ that solves the equation $\dot{\rho} = 0$. If the environment would be absent, $\kappa = 0$, the system would be closed, and the steady states are simply the energy eigenstates of the Hamiltonian. But if instead the Hamiltonian would vanish, $\omega = 0$, the $\hat{S}_-$ operators applied repeatedly on any state, would eventually lead to a pure steady state with the spin pointing down in the z direction. The interesting case is when both the Hamiltonian and the environment are non-zero, a steady state would then arise from a competition of these two, and it is this interplay that renders the phase transition. The aim of this thesis is thus to explore the properties of the steady state of the Lindblad equation, Eq. (1.1). The analytic solution of the model is given as an infinite sum, so an approximation will be calculated numerically for a large spin. From the numerical results, the aspiration is to characterise the type of the phase transition, and to try to find critical exponents. It is also of interest to understand the concept of symmetry breaking in this model since symmetries for an open system has a different meaning than for a closed system [5]. For example, a symmetry of a Lindblad master equation does not automatically imply a conserved quantity, which it always does in the closed case [5].

In the first part of the essay many concepts needed to understand open quantum systems are presented, including the density operator; a representation of a general quantum state, the time evolution in both closed and open systems, and a derivation of the quantum master equation, as well as the theory needed to grasp these ideas. A section on phase transitions is also added, which is however kept very general, to only include necessary knowledge to be able to commence with the solving of the model. The latter part of the thesis consists of the solutions of the steady state, and the exploration of criticality.

2 Beyond pure states

A quantum mechanical state is either a *pure* or *mixed* state [6]. A pure state can always be represented by a vector of the form

$$|\Psi\rangle = \sum_n c_n |\psi_n\rangle. \tag{2.1}$$

Here $|\psi_n\rangle$ forms a complete orthonormal basis, and c_n are complex coefficients such that $|c_n|^2$ is the probability of finding the particle in state $|\psi_n\rangle$ after a measurement of the system has been made. To be able to construct such a vector one must know the magnitude and the relative phase between the coefficients [7]. The representation of a state must be unique regardless of the basis it is presented in; the relative phase must thus be known since the new coefficients, when a change of basis is made, depend on the phase between the old ones.

A pure state is not the most general quantum state. If an ensemble of states are prepared independently from one another, the ensemble is called an statistical mixture, or shorter, a mixed state [7]. A mixed state is thus a statistical distribution of pure states. Since each state has been prepared independently, there cannot exist a defined relative phase difference between the states, and Eq. (2.1) cannot be used to express the state of the ensemble of all the particles [7]. To represent a mixed state the formalism of *density operators* is used, which are explained in the following section [7].

2.1 The Density Operator

In order to give a description for a mixed state, the traditional view of a state as a bra- or a ket-vector must be discarded and instead the density operator,

ρ is introduced and defined as [6]

$$\rho = \sum_n P_n |\psi_n\rangle\langle\psi_n|. \tag{2.2}$$

Here P_n is the statistical weight (i.e. they are real non negative numbers) of each prepared state, and thence

$$\sum_n P_n = 1. \tag{2.3}$$

If only a single probability P_n is non zero there is no statistical distribution and the state is a pure state [6] and has the form

$$\rho = |\psi\rangle\langle\psi|. \tag{2.4}$$

Any of the states $|\psi_n\rangle$ forming the density operator may be expressed in a complete orthonormal basis, $\{|\varphi_\nu\rangle\}$, [7] as follows,

$$|\psi_n\rangle = \sum_{i'} a_{i'}^{(n)} |\varphi_{i'}\rangle \tag{2.5}$$

and

$$\langle\psi_n| = \sum_{j'} a_{j'}^{(n)*} \langle\varphi_{j'}|. \tag{2.6}$$

For any density matrix ρ it is true that ρ is Hermitian, $\rho = \rho^\dagger$, $\rho_{ii} \geq 0$, and $\mathrm{Tr}\rho = 1$ [6]. To check that ρ is Hermitian its matrix elements are calculated:

$$\rho_{ij} = \langle\varphi_i|\rho|\varphi_j\rangle = \langle\varphi_i| \sum_{i'j'n} P_n a_{i'}^{(n)} a_{j'}^{(n)*} |\varphi_{i'}\rangle\langle\varphi_{j'}|\varphi_j\rangle = \sum_n P_n a_i^{(n)} a_j^{(n)*}. \tag{2.7}$$

From above it is clear that $\langle\varphi_i|\rho|\varphi_j\rangle = \langle\varphi_j|\rho|\varphi_i\rangle^*$, which thus shows that ρ is Hermitian. The diagonal elements of the density matrix are

$$\rho_{ii} = \sum_n P_n |a_i^{(n)}|^2, \tag{2.8}$$

where both factors in the sum are probabilities; P_n the probability to find the system in state $|\psi_n\rangle$ and $|a_i^{(n)}|^2$ is the probability that $|\psi_n\rangle$ is in state $|\varphi_i\rangle$ [7]. Therefore Eq. (2.8) is the probability to find the system in state $|\varphi_i\rangle$ [7]. This probability must of course obey $\rho_{ii} \geq 0$.

By using Eq. (2.3), the trace of the density operator is seen to equal one,

$$\mathrm{Tr}\rho = \sum_i \rho_{ii} = \sum_i \sum_n P_n |a_i^{(n)}|^2 = 1, \tag{2.9}$$

and this trace is independent of the basis used [7]. The expectation value $\langle \hat{Q} \rangle$ of an arbitrary operator $\hat{Q}$ for a statistical mixture of states is attained by first calculating the expectation value $\langle \hat{Q}_n \rangle$ of each pure state,

$$\langle \hat{Q}_n \rangle = \langle \psi_n | \hat{Q} | \psi_n \rangle, \tag{2.10}$$

and then summing these terms multiplied by their statistical weights,

$$\langle \hat{Q} \rangle = \sum_n P_n \langle \psi_n | \hat{Q} | \psi_n \rangle = \sum_{nij} P_n a_i^{(n)} a_j^{(n)*} \langle \varphi_j | \hat{Q} | \varphi_i \rangle = \tag{2.11}$$
$$\sum_{ij} \langle \varphi_i | \rho | \varphi_j \rangle \langle \varphi_j | \hat{Q} | \varphi_i \rangle = Tr(\rho \hat{Q}).$$

The *partial trace* is another important concept regarding the density operator. If a system consists of many coupled subsystems, but only one of these is of interest, the others may be *traced out*, by taking the partial trace over all the non-interesting systems [7]. Let $|\varphi_i\rangle$ be the states forming the density matrix representing the system of interest and $|\Phi_j\rangle$ all the other systems, where the $|\Phi_j\rangle$'s are assumed orthogonal. If an operator $\hat{Q}(\varphi)$ only acts on the system of interest, its matrix elements are given by

$$\langle \Phi_{j'} \varphi_{i'} | \hat{Q}(\varphi) | \Phi_j \varphi_i \rangle = \langle \varphi_{i'} | \hat{Q}(\varphi) | \varphi_i \rangle \delta_{jj'}. \tag{2.12}$$

And it follows that

$$\langle \hat{Q}(\varphi, t) \rangle = \mathrm{Tr}(\rho(t) \hat{Q}(\varphi)) = \sum_{ii'} \left(\sum_j \langle \Phi_j \varphi_{i'} | \rho(t) | \Phi_j \varphi_i \rangle \right) \langle \varphi_i | \hat{Q}(\varphi) | \varphi_{i'} \rangle. \tag{2.13}$$

The density matrix of interest is $\rho(\varphi, t)$, which is also called the *reduced density matrix* [7]. Its elements can be defined as

$$\langle \varphi_{i'} | \rho(\varphi, t) | \varphi_i \rangle = \sum_j \langle \Phi_j \varphi_{i'} | \rho(t) | \Phi_j \varphi_i \rangle, \tag{2.14}$$

thus

$$\langle \hat{Q}(\varphi, t) \rangle = \mathrm{Tr}(\rho(\varphi, t) \hat{Q}(\varphi)), \tag{2.15}$$

so when the partial density matrix is known, all properties of the system of interest can be found. If we only have access to the system, i.e. can perform measurements on it, all information we can extract is contained in the reduced density operator. By rewriting Eq. (2.14), as

$$\langle \varphi_{i'} | \rho(\varphi, t) | \varphi_i \rangle = \langle \varphi_{i'} | \left(\sum_j \langle \Phi_j | \rho(t) | \Phi_j \rangle \right) | \varphi_i \rangle, \tag{2.16}$$

it becomes clear that the expression in the brackets is just the partial trace [7], $\mathrm{Tr}_\Phi(\rho(t))$ of $\rho(t)$ with respect to Φ_j, so with this notation

$$\rho(\varphi, t) = \mathrm{Tr}_\Phi(\rho(t)). \tag{2.17}$$

A pure state was defined as a state (Eq. (2.2)) with only a single non zero P_n. However, it is *a priori* usually not clear in which basis the density operator can be written as in Eq. (2.4) and it is thereby desirable to be able to quantify how pure/mixed a state is. To do so, the concept of *purity* is introduced. The purity may be tested by calculating $\mathrm{Tr}(\rho^2)$ [8]. From the expression for the pure state, Eq. (2.1) it is easy to see that $\mathrm{Tr}(\rho^2) = 1$ whenever ρ is pure. In general the purity varies as

$$\frac{1}{N} \leq \mathrm{Tr}(\rho^2) \leq 1, \tag{2.18}$$

where N is the dimension of the system [6]. The lower bond can be verified by diagonalising ρ, which gives $\mathrm{Tr}(\rho^2) = \sum_i^N \lambda_i^2$, where λ_i are the eigenvalues of ρ. With the help of a Lagrangian multiplier the normalisation constraint of ρ is met and ends up minimising the function

$$F(\lambda,\eta) = \sum_i^N \lambda_i^2 + \eta\left(\sum_i^N \lambda_i - 1\right), \tag{2.19}$$

by calculating the partial derivatives and setting them to zero, i.e.

$$\begin{aligned} \partial_{\lambda_i} F &= 2\lambda_i + \eta \equiv 0, \\ \partial_\eta F &= \sum_i^N \lambda_i - 1 \equiv 0. \end{aligned} \tag{2.20}$$

From here it is clear that $\lambda_i = -\eta/2 = c =$ constant, for all values of i and that $\sum_i^N \lambda_i = Nc \implies c = 1/N$. Hence the minimal value of the purity is

$$\mathrm{Tr}(\rho^2)_{min} = \left(\sum_i^N \lambda_i^2\right)_{min} = \frac{N}{N^2} = \frac{1}{N}, \tag{2.21}$$

where $\mathrm{Tr}(\rho^2) = \frac{1}{N}$ implies that the state of the system is maximally mixed. Note that such a state is what one would expect; we have no information about coherences (off diagonal elements of ρ) and each state is equally probable regardless of basis.

3 Time evolution of closed quantum systems

In quantum mechanics one can talk about *closed*- and *open* quantum systems. The definition for a closed systems follows that of Breuer *et al* [4], where closed systems include *isolated* systems; systems where the Hamiltonian is time independent, and *driven* systems; systems driven by an external field and possessing a time dependent Hamiltonian. Open systems are, according to this definition, systems which are coupled to an outside environment. There are different ways or pictures in which the dynamics of a quantum system may be expressed, they are the *Schrödinger, Heisenberg and interaction pictures* which all have their own advantages for different problems [8].

3.1 The Schrödinger picture

In the Schrödinger picture the time evolution is contained in the state of the system, whilst any operators are expressed as time independent [4]. The Schrödinger equation is used to calculate the time evolution of a pure state,

$$i\hbar\frac{\partial|\Psi(t)\rangle}{\partial t} = \hat{H}(t)|\Psi(t)\rangle, \tag{3.1}$$

where the solution may be expressed as a transformation of the state at time $t = t_0$ [4]

$$|\Psi(t)\rangle = \hat{U}(t, t_0)|\Psi(t_0)\rangle. \tag{3.2}$$

$\hat{U}$ is a unitary operator, which can be shown by substituting Eq. (3.2) into the Schrödinger equation and using the initial condition $\hat{U}(t_0, t_0) = I$ [4]. The time evolution of a closed and isolated system is generated by a Hamiltonian, which means that there exists a time independent Hamiltonian, $\hat{H}$, such that the unitary operator can be expressed as $\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t}$ [4]. In fact for any unitary operator there exists a Hermitian operator such that the unitary operator may be expressed as an exponential in this way, and for the time evolution operator this Hermitian operator is the Hamiltonian. The time evolution of a mixed state may therefore be expressed as

$$\rho(t) = \sum_i P_i\hat{U}(t, t_0)|\Psi_i(t_0)\rangle\langle\Psi_i(t_0)|\hat{U}^\dagger(t, t_0) = \hat{U}(t, t_0)\rho(t_0)\hat{U}^\dagger(t, t_0), \tag{3.3}$$

where the normalised vectors $|\Psi_i(t_0)\rangle$ evolve according to Eq. (3.2) [4]. For simplicity of notation, we will set $\hbar = 1$ in all further calculations throughout the thesis. The time derivative of the above equation directly yields the *Liouville- von Neumann equation*,

$$\dot{\rho(t)} = -i[\hat{H}(t), \rho(t)]. \tag{3.4}$$

The Liouville- von Neumann equation thus expresses the time evolution of the density matrix and under such unitary time evolution, mixed states may never be created nor destroyed, a pure/mixed state transforms into another pure/mixed state [7].

3.2 The Heisenberg picture

In the Heisenberg picture the density matrix expressing the state is time independent, instead the time dependency is shifted to the operators [8], which is shown through the unitary transformation

$$\hat{A}_H(t) = \hat{U}^\dagger(t, t_0)\hat{A}(t_0)\hat{U}(t, t_0). \tag{3.5}$$

In the above equation, $\hat{A}_H(t)$ is an operator expressed in the Heisenberg picture, and $\hat{A}(t_0)$ the same operator in the Schrödinger picture. It is assumed that the density operators for both pictures are the same at some initial time $t = t_0$ [4] so Eq. (3.5) implies that the operators also are the same at this time. The equation of motion in the Heisenberg picture is given by taking the total time derivative of Eq. (3.5) *i.e.*

$$\frac{\mathrm{d}\hat{A}_H(t)}{\mathrm{d}t} = i[\hat{H}_H(t), \hat{A}_H(t)] \tag{3.6}$$

where the Hamiltonian, $\hat{H}_H(t)$, in the Heisenberg picture is the same as the Hamiltonian in the Schrödinger picture since it commutes with itself, so it is a constant of motion [8]. The two pictures used to express time evolution in closed quantum systems are equal, which is proven by showing that all expectation values are identical regardless of picture [8], by using the cyclic property of the trace,

$$\begin{aligned} \mathrm{Tr}(\hat{A}_H(t)\rho_H(t_0)) = \mathrm{Tr}(\hat{U}^\dagger(t, t_0)\hat{A}(t_0)\hat{U}(t, t_0)\rho_H(t_0)) = \\ \mathrm{Tr}(\hat{U}(t, t_0)\rho_H(t_0)\hat{U}^\dagger(t, t_0)\hat{A}(t_0)) = \mathrm{Tr}(\rho(t)\hat{A}(t_0)). \end{aligned} \tag{3.7}$$

If a system is driven by an external force, the Hamiltonian may be time dependent, and in this case the operators in the Schrödinger picture may also be time dependent [4], and Eq. (3.6) then contains an extra term so that the equation

$$\frac{\mathrm{d}\hat{A}_H(t)}{\mathrm{d}t} = i[\hat{H}_H(t), \hat{A}_H(t)] + \frac{\partial \hat{A}_H(t)}{\partial t} \tag{3.8}$$

gives the time evolution of an operator in the Heisenberg picture.

3.3 The interaction picture

In the previous two sections the Hamiltonian has (mainly) been regarded as time independent, however, the Hamiltonian may well depend on time, which is why the interaction picture is of particular interest. In the interaction picture the Hamiltonian is considered as two separate parts, a time independent part, $\hat{H}_0$ and a time dependent one, $\hat{V}(t)$, so that the total Hamiltonian of the system is

$$\hat{H}_{IF}(t) = \hat{H}_0 + \hat{V}(t), \tag{3.9}$$

where the subscript IF stands for *interaction frame* [9]. The time dependence of the Hamiltonian may be explicitly removed by defining [7],

$$|\Psi(t)_S\rangle = e^{-i\hat{H}_0 t}|\Psi(t)_{IF}\rangle, \tag{3.10}$$

with the S subscript denoting the Schrödinger picture, and the implicit time dependence is,

$$|\Psi(t)_{IF}\rangle = \sum_n C_n(t)|\psi_n^{(0)}\rangle. \tag{3.11}$$

The states $|\psi_n^{(0)}\rangle$ are the eigenstates of $\hat{H}_0$ and the time dependence of the Hamiltonian is carried within the coefficients $C_n(t)$ [7]. In the interaction picture, the evolution of the system is governed by [7],

$$i\frac{\partial|\Psi(t)_{IF}\rangle}{\partial t} = \hat{V}(t)_{IF}|\Psi(t)_{IF}\rangle, \tag{3.12}$$

where

$$\hat{V}(t)_{IF} = e^{i\hat{H}_0 t}\hat{V}(t)e^{-i\hat{H}_0 t}. \tag{3.13}$$

In fact, all operators $\hat{Q}(t)$ may be transformed in this way [7],

$$\hat{Q}(t)_{IF} = e^{i\hat{H}_0 t}\hat{Q}(t)e^{-i\hat{H}_0 t}. \tag{3.14}$$

Table 3 summarises the three pictures and how the time evolution is carried out.

	Heisenberg picture	Interaction picture	Schrödinger picture
State	No change	Evolution determined by $\hat{V}(t)$	Evolution determined by $\hat{H}(t_0)$
Operator	Evolution determined by $\hat{H}(t_0)$	Evolution determined by $\hat{H}_0$	No change

Table 1: A comparison of the Heisenberg, interaction, and Schrödinger pictures with respect to where the time dependence lies [9].

By using Eq. (3.10) the interaction picture state may be expressed in terms of the state in the Schrödinger picture

$$|\Psi(t)_{IF}\rangle = e^{i\hat{H}_0 t}|\Psi(t)_S\rangle) = e^{i\hat{H}_0 t}\hat{U}(t,0)|\Psi(0)_S\rangle). \tag{3.15}$$

At time $t = 0$ we have that

$$|\Psi(0)_{IF}\rangle = |\Psi(0)_S\rangle, \tag{3.16}$$

so the state in the interaction picture is

$$|\Psi(t)_{IF}\rangle = \hat{U}_{IF}(t,0)|\Psi(0)_{IF}\rangle, \tag{3.17}$$

where we have defined

$$\hat{U}_{IF}(t,0) = e^{i\hat{H}_0 t}\hat{U}(t,0). \tag{3.18}$$

However, often the expression for $\hat{U}(t,0)_{IF}$ is simplified by letting $\hat{U}_{IF}(t,0) = \hat{U}(t,0)$[1] [8]. This simplification is referred to as *working in the interaction frame*, and one can thus express the Schrödinger and Heisenberg pictures in this frame [8]. The Heisenberg picture in the interaction frame has the form

$$\rho(t) = \rho(0), \qquad \hat{A}(t) = \hat{U}^{\dagger}_{IF}(t,t_0)\hat{A}(0)\hat{U}_{IF}(t,t_0) \tag{3.19}$$

and correspondingly, the Schrödinger picture in the interaction frame has the form

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[1] This simplification is motivated by the fact that $\hat{V}_{IF}$ may often be made time-independent either by a clever choice of division of the total Hamiltonian into $\hat{H}_0$ and $\hat{V}$, or by using a motivated approximation [8].

$$\rho(t) = \hat{U}^{\dagger}_{IF}(t,t_0)\rho(0)\hat{U}_{IF}(t,t_0), \quad \hat{A}(t) = \hat{A}(0). \tag{3.20}$$

It is important to notice this difference between the interaction picture, with the full Hamiltonian evolution and the interaction frame, in which the simplification of the unitary operator is made [8].

4 Time evolution of open quantum systems

An open quantum system is a system which is coupled to an environment, as defined in section 3 [4]. The combined system, system+environment, is often considered a closed system, so also in this thesis. The time evolution of the combined system is hence Hamiltonian, and could in theory be solved with a unitary transformation. However, in practise the dynamics of the combined system is too complicated to solve, at least in physically important models, which is why it is of interest to look at the system of interest as open. [4] The open system, on the other hand, interacts with the environment which leads to correlations between the system and the environment which results in a non unitary time evolution for the system alone [4]. The solutions for the open system may be achieved by tracing out the environment, but this in turn means that one must work with non unitary equations of motion. Such an equation is called a *quantum master equation*, and it is derived utilising appropriate approximations for the model used [4]. Fig. (1) shows a schematic diagram depicting the time evolution.

$$\begin{tikzcd}
\rho(t_0) = \rho_S(t_0) \otimes \rho_E(t_0) \arrow[r, "\text{unitary evolution}"] \arrow[d, "\mathrm{Tr}_E"] & \rho(t) = \hat{U}[\rho_S(t_0) \otimes \rho_E(t_0)]\hat{U}^{\dagger} \arrow[d, "\mathrm{Tr}_E"] \\
\rho_S(t_0) \arrow[r, "\text{quantum master equation}"] & \rho_S(t)
\end{tikzcd}$$

Figure 1: A schematic diagram which shows the action of a quantum master equation [4]. As the trace is an irreversible operation, the time evolution of the system cannot be unitary, i.e. the lower horizontal time arrow cannot be reversed.

4.1 Derivation of the Born-Markov master equation

Under certain circumstances, the time evolution for an open system can be described by the *Born-Markov master equation* [8]. In this model the open system is coupled with a large bath, so that the system and the bath together make up a closed system [8]. It is assumed that the coupling between the two is weak, which implies that the system does not significantly affect the bath. This approximation is called the *Born approximation* [8]. It is also assumed that that the bath does not have any memory of past events, due to it being so large compared to the system, which can be thought of as if the system interacts with a different part of the bath at each moment. This is called the *Markov approximation* [8].

The Hamiltonian for the total system is

$$\hat{H}_{S+E} = \hat{H}_S + \hat{H}_E + \hat{V}, \tag{4.1}$$

where the first two terms are the Hamiltonians for the system and the environment respectively, and $\hat{V}$ the Hamiltonian expressing the coupling between the two [8]. The time evolution for the total system is therefore according to the Liouville von Neumann equation,

$$\dot{\rho}_{tot}(t) = -i[\hat{H}_S + \hat{H}_E + \hat{V}, \rho_{tot}(t)]. \tag{4.2}$$

The derivation of the master equation proceeds in the interaction frame in which the above equation has the form

$$\dot{\rho}_{tot_{IF}}(t) = -i[\hat{V}_{IF}(t), \rho_{tot_{IF}}(t)]. \tag{4.3}$$

This differential equation may be solved itteratively [8] and integration yields

$$\rho_{tot_{IF}}(t) = \rho_{tot_{IF}}(0) - i\int_0^t \mathrm{d}t'[\hat{V}_{IF}(t'), \rho_{tot_{IF}}(t')]. \tag{4.4}$$

Next $\rho_{tot_{IF}}(t)$ from Eq. (4.3) is substituted with this first degree itteration and the equation now reads

$$\dot{\rho}_{tot_{IF}}(t) = -i[\hat{V}_{IF}(t), \rho_{tot_{IF}}(0)] - \int_0^t \mathrm{d}t'[\hat{V}_{IF}(t), [\hat{V}_{IF}(t'), \rho_{tot_{IF}}(t')]]. \tag{4.5}$$

The environment is then traced out, to acquire a solution for the open system [8]. The first term disappears since $\mathrm{Tr}_E[\hat{V}_{IF}(t), \rho_{tot_{IF}}(0)] = 0$. This is always true since $\hat{V}_{IF}$ depends on $\hat{V}$ and the latter always can be defined so that the partial trace of the first term is zero [10], so we are left with

$$\dot{\rho}_{S_{IF}}(t) = -\int_0^t \mathrm{d}t' \mathrm{Tr}_E[\hat{V}_{IF}(t), [\hat{V}_{IF}(t'), \rho_{tot_{IF}}(t')]]. \tag{4.6}$$

In the following step the Born approximation is used to simplify this expression. Since it is now assumed that the interaction has an insignificant effect on the environment, the density matrix of the combined system may be expressed with the tensor product [4]

$$\rho_{tot_{IF}}(t) = \rho_{S_{IF}}(t) \otimes \rho_{E_{IF}}(0), \tag{4.7}$$

which when substituted into Eq. (4.6) gives the expression

$$\dot{\rho}_{S_{IF}}(t) = -\int_0^t \mathrm{d}t' \mathrm{Tr}_E[\hat{V}_{IF}(t), [\hat{V}_{IF}(t'), \rho_{S_{IF}}(t') \otimes \rho_{E_{IF}}(0)]]. \tag{4.8}$$

Now the Markov approximation will be used twice, allowing us to greatly simplify the equation. First the equation is made local in time by replacing $\rho_{S_{IF}}(t')$ with $\rho_{S_{IF}}(t)$ inside the integral, which is justified as long as the integral goes to zero apart from when $t \approx t'$ [8]. This means that the equation only depends on the present state of the density matrix, and the approximation depends on the fact that the bath lacks memory of past events [8]. The resulting equation

$$\dot{\rho}_{S_{IF}}(t) = -\int_0^t \mathrm{d}t' \mathrm{Tr}_E[\hat{V}_{IF}(t), [\hat{V}_{IF}(t'), \rho_{S_{IF}}(t) \otimes \rho_{E_{IF}}(0)]] \tag{4.9}$$

is called the *Redfield equation*. The last step uses the Markov approximation to eliminate the explicit dependence on the choice of starting time of the time evolution of the density matrix. This is done by extending the lower limit of the integral in Eg.(4.9) to minus infinity. This is again motivated by the assumption that the integrand is sharp around $t' \approx t$ and very small otherwise [8]. This then gives

$$\dot{\rho}_{S_{IF}}(t) = -\int_{-\infty}^t \mathrm{d}t' \mathrm{Tr}_E[\hat{V}_{IF}(t), [\hat{V}_{IF}(t'), \rho_{S_{IF}}(t) \otimes \rho_{E_{IF}}(0)]], \tag{4.10}$$

which is the final expression for the Born-Markov master equation.

4.2 The Lindblad equation

The most general form of the Born-Markov master equation is the *Lindblad equation* [10]. The Lindblad equation expressed in the Schrödinger picture has the form

$$\dot{\rho}(t) = -i[\hat{H}_S, \rho(t)] + \kappa \sum_j \left\{ \hat{L}_j \rho(t) \hat{L}_j^\dagger - \frac{1}{2}\left(\hat{L}_j^\dagger \hat{L}_j \rho(t) + \rho(t) \hat{L}_j^\dagger \hat{L}_j \right) \right\} \tag{4.11}$$

where $\hat{H}_S$ is the system Hamiltonian, and the operators $\hat{L}$ are called Lindblad operators and they represent the influence the environment has on the system [10]. Here the derivation of the Lindblad equation will be performed by looking at spontaneous emission in a system with two energy levels where the environment consists of an electromagnetic field. For such a system the Hamiltonian of the environment is given by a set of harmonic oscillators

$$\hat{H}_E = \sum_k \omega_k \hat{a}_j^\dagger \hat{a}_k, \tag{4.12}$$

with frequency ω_k, and k being the mode of the electromagnetic field; it contains the information of the polarisation, frequency, transverse structure and direction [8]. The operators $\hat{a_k}$ and $\hat{a}_j^\dagger$ are the annihilation and creation operators which obey the commutation relation

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}. \tag{4.13}$$

The system Hamiltonian, $\hat{H}_S$ of this model consists of the frequency difference, ω_a of the ground and exited state of the atom, and $\hat{\sigma}_z = |1\rangle\langle 1| - |0\rangle\langle 0|$, which is one of the Pauli operators, so the Hamiltonian has the form [8]

$$\hat{H}_S = \frac{\omega_a}{2}\hat{\sigma}_z. \tag{4.14}$$

The Hamiltonian $\hat{V}$ describing the coupling between the system and the environment is in this model given as

$$\hat{V} = \sum_k (g_k \hat{a}_k + g_k \hat{a}_k^\dagger) \left(\hat{\sigma}_+ + \hat{\sigma}_- \right), \tag{4.15}$$

where the first factor of the product in each term of the sum only affects the environment and the other factors only affect the system [8]. $\hat{\sigma}_+$ and $\hat{\sigma}_-$ are the atomic raising and lowering operators, and g_k are real constants which are proportional to the inverse square root of the physical volume of the mode [8]. To proceed, the coupling Hamiltonian is expressed in the interaction frame,

$$\hat{V}_{IF} = e^{i(\hat{H}_E+\hat{H}_S)t}\left(\sum_k (g_k\hat{a}_k + g_k\hat{a}_k^\dagger)\,(\hat{\sigma}_+ + \hat{\sigma}_-)\right)e^{-i(\hat{H}_E+\hat{H}_S)t} = \tag{4.16}$$

$$= \sum_k e^{i\omega_k\hat{a}_k^\dagger\hat{a}_k t}(g_k\hat{a}_k + g_k\hat{a}_k^\dagger)e^{-i\omega_k\hat{a}_k^\dagger\hat{a}_k t}e^{i\frac{\omega_a}{2}\hat{\sigma}_z t}(\hat{\sigma}_+ + \hat{\sigma}_-)e^{-i\frac{\omega_a}{2}\hat{\sigma}_z t} =$$

$$\left[\text{Let, } \hat{A}_k = e^{-i\omega_k\hat{a}_k^\dagger\hat{a}_k t},\ \ \hat{B}_k = e^{-i\frac{\omega_a}{2}\hat{\sigma}_z t}.\right]$$

$$= \sum_k (g_k\hat{A}^\dagger\hat{a}_k\hat{A} + g_k\hat{A}^\dagger\hat{a}_k^\dagger\hat{A})(\hat{B}^\dagger\hat{\sigma}_+\hat{B} + \hat{B}^\dagger\hat{\sigma}_-\hat{B}).$$

This expression may be further simplified. Consider the equation

$$a(t)_k = \hat{A}_k^\dagger\hat{a}_k\hat{A}_k. \tag{4.17}$$

By taking the time derivative of both sides of Eq. (4.17), and using that any operator commutes with its exponential[2] it can be shown with the use of commutator relations that

$$\dot{a}(t)_k = -i\omega_k a(t)_k. \tag{4.18}$$

But the solution of this first order differential equation is

$$a(t)_k = e^{-i\omega_k t}a(0)_k = e^{-i\omega_k t}\hat{a}_k. \tag{4.19}$$

By approaching the other factors in each bracket of Eq. (4.16) in the same manner the coupling potential may be written as

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[2] This follows from the definition of $e^{\hat{Q}t}$ as the Taylor expansion $e^{\hat{Q}t} = \hat{1} + \hat{Q}t + \frac{\hat{Q}^2}{2!}t^2....$

$$\hat{V}_{IF} = \sum_k (g_k e^{-i\omega_k t} \hat{a}_k + g_k e^{i\omega_k t} \hat{a}_k^\dagger)(e^{i\omega_a t}\hat{\sigma}_+ + e^{-i\omega_a t}\hat{\sigma}_-). \tag{4.20}$$

At this point the *rotating wave approximation* is employed. In this approximation all exponents with $\omega_k + \omega_a$ are removed; these terms are rotating in the complex plane with such high frequency in comparison to the frequency of the radiative decay from the exited to the ground state, that their average is zero [8], so the final expression for the coupling is hence

$$\hat{V}_{IF} = \sum_k \left(g_k \hat{a}_k \hat{\sigma}_+ e^{-i(\omega_k - \omega_a)t} + g_k \hat{a}_k^\dagger \hat{\sigma}_- e^{i(\omega_k - \omega_a)t} \right). \tag{4.21}$$

To continue the derivation, the above expression for the coupled Hamiltonian is inserted into the Redfield equation, Eq. (4.9), and the commutators within the integral are expanded, which will result in 16 terms per mode. If the environments ground state is defined to be the vacuum[3] state [10],

$$\rho_{E_{IF}}(0) = |0_{b1}\rangle\langle 0_{b1}| \otimes |0_{b2}\rangle\langle 0_{b2}| \otimes ... \tag{4.22}$$

it can be verified that

$$\sum_{kk'} \mathrm{Tr}_E(\hat{a}_{k'}\hat{a}_k \rho_{E_{IF}}(0)) = \sum_{kk'} \mathrm{Tr}_E(\hat{a}_{k'}^\dagger \hat{a}_k^\dagger \rho_{E_{IF}}(0)) = 0. \tag{4.23}$$

So half of the 16 terms will become zero when the environment is traced out. For a more compact notation let us define

$$\hat{C}(t) = e^{-i((\omega_k - \omega_a)t}. \tag{4.24}$$

The density operator is to be understood to be in the Schrödinger picture, working in the interaction frame, even though the subscript IF will be dropped in the following calculations. By using the cyclic property of the trace on the remaining terms the integrand in Eq. (4.9) is

$$\mathrm{Tr}_E[\hat{V}(t), [\hat{V}(t'), \rho_S(t) \otimes \rho_E(0)]] = \tag{4.25}$$

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[3] The vacuum state is the state with lowest energy and containing no particles [11]. For interactions among the particles it may happen, though, that the ground state is not the vacuum.

$$\sum_{k,k'} g_k g_{k'} [(\hat{\sigma}_+\hat{\sigma}_-\rho_S - \hat{\sigma}_-\rho_S\hat{\sigma}_+)\mathrm{Tr}_E(\hat{a}_k\hat{a}^\dagger_{k'}\rho_E)\hat{C}(t)\hat{C}^\dagger(t')$$

$$+(\rho_S\hat{\sigma}_-\hat{\sigma}_+ - \hat{\sigma}_+\rho_S\hat{\sigma}_-)\mathrm{Tr}_E(\hat{a}^\dagger_{k'}\hat{a}_k\rho_E)\hat{C}(t)\hat{C}^\dagger(t')$$

$$+(\hat{\sigma}_-\hat{\sigma}_+\rho_S - \hat{\sigma}_+\rho_S\hat{\sigma}_-)\mathrm{Tr}_E(\hat{a}^\dagger_{k}\hat{a}_{k'}\rho_E)\hat{C}^\dagger(t)\hat{C}(t')$$

$$+(\rho_S\hat{\sigma}_+\hat{\sigma}_- - \hat{\sigma}_-\rho_S\hat{\sigma}_+)\mathrm{Tr}_E(\hat{a}_{k'}\hat{a}^\dagger_{k}\rho_E)\hat{C}^\dagger(t)\hat{C}(t')].$$

The remaining expressions of the partial traces are evaluated as follows,

$$\sum_{ij}\mathrm{Tr}_E(\hat{a}^\dagger_i\hat{a}_j\rho_E) = \sum_{ij}\sum_b\langle b|\hat{a}^\dagger_i\hat{a}_j(|0_{b1}\rangle|0_{b2}\rangle...)(\langle 0_{b1}|\langle 0_{b2}|...)|b\rangle = \tag{4.26}$$

$$(\langle 0_{b1}|\langle 0_{b2}|...)\sum_b|b\rangle\langle b|\sum_{ij}\hat{a}^\dagger_i\hat{a}_j(|0_{b1}\rangle|0_{b2}\rangle...) =$$

$$(\langle 0_{b1}|\langle 0_{b2}|...)\sum_{ij}\hat{a}^\dagger_i\hat{a}_j(|0_{b1}\rangle|0_{b2}\rangle...) = 0,$$

where $|b\rangle$ is a complete basis of the environment, and also

$$\sum_{k,k'} g_k g_{k'}\hat{C}(t)\hat{C}^\dagger(t')\mathrm{Tr}_E(\hat{a}_k\hat{a}^\dagger_{k'}\rho_E) \tag{4.27}$$

$$= \sum_{k,k'} g_k g_{k'}\hat{C}(t)\hat{C}^\dagger(t')\sum_b\langle b|\hat{a}_k\hat{a}^\dagger_{k'}(|0_{b1}\rangle|0_{b2}\rangle...)(\langle 0_{b1}|\langle 0_{b2}|...)|b\rangle$$

$$= \sum_{k,k'} g_k g_{k'}\hat{C}(t)\hat{C}^\dagger(t')(\langle 0_{b1}|\langle 0_{b2}|...)\sum_b|b\rangle\langle b|\hat{a}_k\hat{a}^\dagger_{k'}(|0_{b1}\rangle|0_{b2}\rangle...)$$

$$= \sum_{k,k'} g_k g_{k'}\hat{C}(t)\hat{C}^\dagger(t')(\langle 0_{b1}|\langle 0_{b2}|...)\hat{a}_k\hat{a}^\dagger_{k'}(|0_{b1}\rangle|0_{b2}\rangle...)$$

$$= \Big[\text{ invoking the commutation relation } \quad [\hat{a}_i, \hat{a}^\dagger_j] = \delta_{ij}.\Big]$$

$$= \sum_{k,k'} g_k g_{k'} e^{-i((\omega_k-\omega_a)t-(\omega_{k'}-\omega_a)t')}\delta_{kk'}(\langle 0_{b1}|\langle 0_{b2}|...)(|0_{b1}\rangle|0_{b2}\rangle...)$$

$$+\sum_{k,k'} g_k g_{k'} e^{-i((\omega_k-\omega_a)t-(\omega_{k'}-\omega_a)t')}(\langle 0_{b1}|\langle 0_{b2}|...)\hat{a}^\dagger_{k'}\hat{a}_k(|0_{b1}\rangle|0_{b2}\rangle...)$$

$$= \sum_k g_k^2 e^{-i(\omega_k-\omega_a)(t-t')}.$$

The remaining trace is calculated in the same manner and by using equations (4.26) and (4.27) to simplify Eq. (4.25) the expression for the Redfield equation becomes

$$\dot{\rho} = -\int_0^t \mathrm{d}t' \left(\sum_k g_k^2 e^{-i(\omega_k - \omega_a)(t-t')} (\hat{\sigma}_+ \hat{\sigma}_- \rho_S - \hat{\sigma}_- \rho_S \hat{\sigma}_+) + \mathrm{H.c.} \right), \quad (4.28)$$

where H.c. stands for the Hermitian conjugate term. At this point the Markov approximation is used, but first let us simplify the notation and define

$$\Delta\omega_k = \omega_k - \omega_a, \quad (4.29)$$

and define

$$F(t) = \int_0^t \mathrm{d}t' \left(\sum_k g_k^2 \, e^{-i\Delta\omega_k (t-t')} \right) \quad (4.30)$$

Since the coefficients $g_k \propto \frac{1}{\sqrt{V}}$, where V is the volume of each mode and since an atom in free space has an infinite number of modes witch are all infinite in volume, [8] the terms g_k^2 are infinitesimal, so the sum over the modes may be replaced by an integral over all frequencies of the density of states $J(\omega)$, which is defined as [10],

$$J(\omega) = \sum_k g_k^2 \, \delta(\omega - \Delta\omega_k). \quad (4.31)$$

Also by substituting $\tau = t - t'$, $\mathrm{d}\tau = -\mathrm{d}t'$, $F(t)$ has the form

$$F(t) = \int_0^t \mathrm{d}\tau e^{-i\omega\tau} \int_0^\infty \mathrm{d}\omega J(\omega). \quad (4.32)$$

Now the Markov approximation is applied by letting $t \longrightarrow \infty$ in the time integral which is oscillating, hence it may be calculated by

$$\int_0^\infty \mathrm{d}\tau e^{-i\omega\tau} = \frac{1}{2} \int_{-\infty}^\infty \mathrm{d}\tau e^{-i\omega\tau} = \frac{1}{2} \cdot 2\pi\delta(\omega), \quad (4.33)$$

and thus

$$F = \pi \int_0^\infty \mathrm{d}\omega J(\omega)\delta(\omega), \tag{4.34}$$

which is renamed as $F = \frac{\kappa}{2}$ to reach a more familiar form in the resulting Lindblad equation [10]. Thus, the Lindblad equation in the interaction frame, Eq. (4.10) and Eq. (4.28), is therefore

$$\dot{\rho}_{IF}(t) = \kappa \left[\hat{\sigma}_- \rho_{IF}(t) \hat{\sigma}_+ - \frac{1}{2} \left(\hat{\sigma}_+ \hat{\sigma}_- \rho_{IF}(t) + \rho_{IF}(t) \hat{\sigma}_+ \hat{\sigma}_- \right) \right] \tag{4.35}$$

and transferring back to the Schrödinger picture by using the transformation Eq. (3.20) on both sides of Eq. (4.35) gives

$$\mathrm{LHS} = e^{i\hat{H}_S t} i[\hat{H}_S, \rho] e^{-i\hat{H}_S t} + e^{i\hat{H}_S t} \dot{\rho}\, e^{-i\hat{H}_S t} \tag{4.36}$$

and

$$\mathrm{RHS} = e^{i\hat{H}_S t} \kappa \left[\hat{\sigma}_- \rho\, \hat{\sigma}_+ - \frac{1}{2} \left(\hat{\sigma}_+ \hat{\sigma}_- \rho + \rho\, \hat{\sigma}_+ \hat{\sigma}_- \right) \right] e^{-i\hat{H}_S t}, \tag{4.37}$$

which leads to the Lindblad equation

$$\dot{\rho}_S = -i[\hat{H}_S, \rho] + \kappa \left[\hat{\sigma}_- \rho\, \hat{\sigma}_+ - \frac{1}{2} \left(\hat{\sigma}_+ \hat{\sigma}_- \rho + \rho\, \hat{\sigma}_+ \hat{\sigma}_- \right) \right]. \tag{4.38}$$

To simplify the derivation of the equation, it was commenced with respect to a special case, a harmonic oscillator potential, for which the sum of Lindblad operators in Eq. (4.11) yields only one term. This is also the form for the Lindblad equation for the model considered in this thesis, although, it consists of a different Hamiltonian and Lindblad operator. The derivation is thus enough for the purpose of this thesis but can be generalised using other methods to reach the most general form as shown by Lindblad [4].

5 Phase transitions

We can imagine that a system which exhibits a set of macroscopic quantities, such as density or magnetisation, may be divided into smaller pieces that all have the same properties as the original system. But when the pieces are made small enough they no longer have the same magnetisation nor density, nor any other possible macroscopic quality [1]. The point where this loss happens is connected with the *correlation length* of the system; a measure of the distance over which the particles that make up the system in question are correlated [1]. The correlation length for a system is dependent on external conditions, for example temperature and pressure [1]. Thus, if a system is halved at a distance longer than the correlation length, it does not change the properties of the material since it does not make any difference to the non-correlated particles if the connection is cut between them. In other words, as long as the size of our new smaller system is large in comparison to the correlation length we expect the global properties to remain.

A system that is characterized by a set of macroscopic properties is said to be in a certain *phase*. The concept of a set phase is only really valid when the system becomes infinitely large, since in this limit any fluctuations away from the macroscopic state are very unlikely to occur, and it is thus possible to say that it has a specific set of properties [2]. This limit is called the *thermodynamic limit*, and may be defined as

$$\lim_{N,V\to\infty} \frac{N(\Omega)}{V(\Omega)} = \text{constant}, \tag{5.1}$$

where Ω is the region of the sample, N the number of particles in this region, and V its volume [2]. A system may suddenly change its macroscopic behaviour, when external conditions, such as temperature, is continuously varied and the point where this happens is called a *critical point*; the change itself a *phase transition* [1]. Again, to talk about a phase transition only makes sense when the system is considered in the thermodynamic limit. Phase transitions are often divided into three categories[4], *first order phase transitions*, also called *discontinuous phase transitions*, and *continuous phase transitions* which are sometimes called *second order phase transitions* due to older classification systems and *Kosterlitz-Thoules transitions*, these transitions are continuous at the critical point, as are all its derivatives [2].

A first order phase transition is characterised by a discontinuity of the macroscopic quantities when passing the critical point. This discontinuity arises since the stable phases on each side of the critical point co-exists at the critical point, each of them connected to their respective phase in a close proximity

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[4] There exists more categories, such as 3rd and 4th order transitions, but these are very uncommon [2]. These cannot be characterized by a local order parameter [2].

away from the critical point [1]. The correlation length of first order phase transitions is often finite [1]. Examples of first order phase transitions include the melting of matter and condensation of a gas to a liquid.

For continuous phase transitions the correlation length becomes infinite at the critical point, which implies that the different phases must merge into one at the critical point [1]. The different macroscopic quantities for all the phases go to zero in a smooth fashion when the critical point is approached [1]. An example of a continuous phase transitions is the onset of magnetisation in a ferromagnet when the temperature is varied. Regarding continuous phase transitions, *universality classes* are used; it has been seen that the properties around a critical points are not dependent on the microscopic interactions of the particles in the system, but are rather due to global effects, including for example symmetry properties of the Hamiltonian [1]. This universality means that several systems consisting of different particles will exhibit the same type of behaviour in the vicinity of the critical points, when put under the same global features.

The idea of *Critical exponents* is a feature which only depends on the underlying universality class; the behaviour of thermodynamic quantities in near proximity to a critical point may often be explained with a power law depending on the distance away from the critical point. [12]. These power laws are often said to be *scale free*, which means that it should not matter which scale they are in, they should always be be the same [12]. As an example one can look at the phase transition when a simple liquid is vaporised. Although the critical temperature, T_c for when this happen is different for different elements, the density difference between the two phases for these elements goes to zero according to the same power law, namely $|T_c - T|^{1/3}$, where the critical exponent in this case is 1/3 [12]. So critical exponents are invariant, the system looks the same whatever the scale, and the microscopic details may be overlooked and only the macroscopic details play any role for the critical behaviour of the system [12].

5.1 Spontaneous symmetry breaking

A common phenomena closely related to continuous phase transitions is that of *spontaneous symmetry breaking* [1]. As the name suggests a system may go from being symmetric with respect to an *order parameter*[5] on one side of

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[5] Order parameters contain information about the phase and varies smoothly from being zero above the critical point to becoming non zero below the critical point [2].

the critical point, to becoming asymmetric on the other side of the critical point [1]. The idea of symmetry breaking is especially transparent in the *Landau theory* of phase transitions. Here the Landau free energy, L, is expected to be consistent with the symmetries of the system and be expressible as a power series of its order parameters, η [2]. The spontaneous symmetry breaking can be seen when the free energy is given as a function of a order parameter, and when any external field $H = 0$. As shown in Fig. 2, the system has one minima at $\eta = 0$ when $T > T_c$, and when $T = T_c$ the function has no curvature around, $\eta = 0$. When $T < T_c$ the energy displays two degenerate minima, symmetrical with respect to $+\eta \leftrightarrow -\eta$, where the coordinate of η depends on the temperature [2]. The actual symmetry breaking is reflected in that below the critical point the system spontaneously chooses one of the two minima.

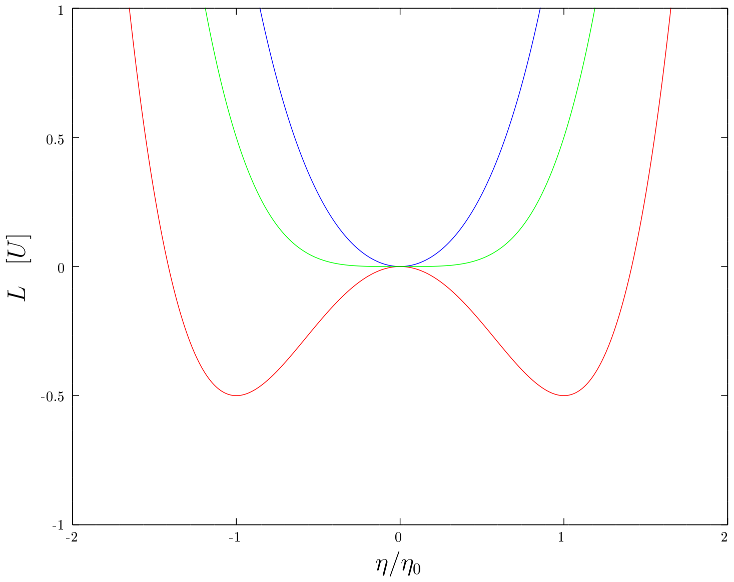

Figure 2: The Landau free energy, L as a function of an arbitary relative order parameter, η/η_0 for the system. The external field $H = 0$. The free energy function behaves differently with respect to the temperature, T, relative to the critical temperature, T_c. The blue graph, for which $T > T_c$ has only one minima, the green graph, $T = T_c$, has no curvature around $\eta = 0$ and the red graph, for $T < T_c$ has two minima, separated by a maxima [2].

An interesting observation is that the behaviour of the above example follows that of a *supercritical pitchfork bifurcation*[6] The name of the bifurcation is understood when the order parameter values at the fixed points of the energy are plotted against the temperature as shown in Fig. 3. The result resembles that of a pitchfork, as T increases a single stable solution is divided into three solutions, two stable symmetrical solutions with an unstable solution between them; this kind of bifurcation is often seen in continuous phase transitions [13].

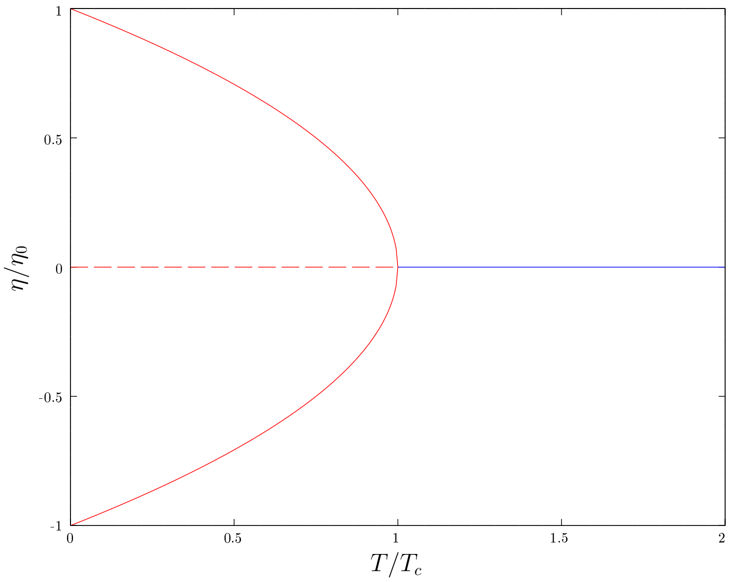

Figure 3: The relative order parameter, η/η_0, for the system as a function of the relative temperature, T/T_c. When the critical temperature, $T = T_c$, is passed from higher to lower T, the symmetry of the system is broken. Here the different colours alude to different solutions according to colour, blue: $T > T_c$ and red: $T < T_c$. This is what is usually called a supercritical pitchfork bifurcation [13].

6 The model

The model that is considered in this thesis consists of a set of N identical atoms, each mimicked here by a two-level system (each level representing an

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[6] Bifurcations are the name of the change of dynamics of fixed points; their creation/disappearance or their change of stability, with respect to a parameter which is varied [13].

internal electronic Zeeman level), which are driven by a resonant external classical field [14]. The system is assumed to be Markovian and this together with the rotating wave approximation imply that the Lindblad equation may be used to describe the dynamics of the system. The Lindblad equation generating the time evolution of the system is taken as

$$\dot{\rho} = -i\left[\omega \hat{S}_x, \rho\right] + \frac{\kappa}{s}\left(2\hat{S}_-\rho\hat{S}_+ - \hat{S}_+\hat{S}_-\rho - \rho\hat{S}_+\hat{S}_-\right). \tag{6.1}$$

Here the Hamiltonian consists of the product between the *Rabi* frequency ω and the collective spin operator

$$\hat{S}_x = \sum_j^N \hat{S}_{x_j}, \tag{6.2}$$

with the spin quantum number of the system, s defined as $s = \frac{N}{2}$ [15]. The term $\hat{S}_{x_j}$ in the sum represents the spin operator for the j:th atom in the system, and the collective spin operators for the y and z components of the spin as well as the collective raising and lowering operators are defined in an analogous manner [11]. The Rabi frequency is the frequency of the oscillation between the two levels caused by the external field [8]. The Lindblad operator is the collective lowering spin operator $\hat{S}_- = \sum_j \hat{S}_{-_j}$, and κ is the Einstein A-coefficient of each atom, for spontaneous emission [15]. It is divided by s to give a correct behaviour in the thermodynamic limit, so that all terms scale as $\sim s$ when N is large. With the introduction of the large spin operator $\hat{S}_z = \sum_j^N \hat{S}_{z_j}$ the following commutation relations hold [14],

$$[\hat{S}_+, \hat{S}_-] = 2\hat{S}_z, \quad [\hat{S}_z, \hat{S}_\pm] = \pm\hat{S}_\pm, \tag{6.3}$$

which follows from the definition

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y. \tag{6.4}$$

The square of the total angular momentum operator, $\hat{S}^2$, of the system is conserved and it is therefore convenient to introduce a set of basis states which are eigenstates to both $\hat{S}^2$ and $\hat{S}_z$ [16]. These are the so called *Dicke states*, a set of basis states for a set of N two level atoms expressed with the simultaneous eigenstates $|l, m\rangle$ of the collective spin operators $\hat{S}^2$ and $\hat{S}_z$ such that [11]

$$\hat{S}^2|l,m\rangle = l(l+1)|l,m\rangle, \tag{6.5}$$

$$\hat{S}_z|l,m\rangle = m|l,m\rangle.$$

For a system with N_1 atoms in the ground state and N_2 atoms in the exited state, m is defined as

$$m = \frac{1}{2}(N_2 - N_1), \tag{6.6}$$

and hence takes integer or half integer values in the interval $-\frac{N}{2} \leq m \leq \frac{N}{2}]$ [11]. l is called the cooperation number and takes values in the interval $|m| \leq l \leq \frac{N}{2}$ [11].

Before the external field is switched on, it may be assumed that all atoms are in the ground state at time $t = 0$ [16]. We then have $m = -\frac{N}{2}$ and $l = \frac{N}{2}$ and remembering that $s = \frac{N}{2}$, it follows that the density matrix expressing the dynamics of the system has dimension $(2s+1) \times (2s+1)$ [16]. The possible collective atomic states are $|\frac{N}{2}, m\rangle$, and to simplify notation by the variable substitution $p = s - m$, and relabel the state $|s, s-p\rangle$ as $|p\rangle$ [16]. Eq. (6.5) is rewritten in this notation as

$$\hat{S}^2|p\rangle = s(s+1)|p\rangle \tag{6.7}$$

$$\hat{S}_z|p\rangle = (s-p)|p\rangle.$$

Since a collective spin for the system is introduced, one large spin $s = \frac{N}{2}$ is considered rather than a collection of N spin half particles, the system only has one effective degree of freedom, and one total spin. Hence the size of *quantum fluctuations*[7], ds, with respect to s, $K = \frac{\mathrm{d}s}{s}$, goes to zero for large s, and the system should behave like a classical system for large collective spin s. This would represent the classical limit for a quantum spin. The system will be solved for in its steady state for general N. In the following sections both a *mean-field approximation* and a numerical approximation of the exact solution for the steady state will be presented and discussed.

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[7] Quantum fluctuations will be explained in the next subsection.

6.1 Mean-field solution for the steady state

Most models of interacting systems are not solvable analytically, and approximative methods are needed. A type of simple approximative methods used are collected under the name *Mean-field theory*, where the behaviour of statistical systems is investigated by simplifying a many-body problem into a one body problem; a much simpler problem to solve [12]. This is achieved by replacing the interactions from all other components in a system upon one of the components with average interaction of these components [17]. This method of replacing by the average implies that a mean field model is more accurate if the system observed consists of a large number of particles.

Mean-field theory also ignores *quantum fluctuations* of the observed quantity, hence it is a bad approximation for systems with large fluctuations, whilst giving a more accurate model of systems with small or insignificant fluctuations [12]. These quantum fluctuations derive from the Heisenberg uncertainty principle; since non commuting operators do not have simultaneous eigenstates, there will always be an uncertainty regarding their physical properties [9]. In the approximation, non-commuting operators are replaced with commuting ones [17]. The corrections for this replacement scales as $\frac{1}{N}$, where N is the number of particles, hence it matters less for large systems when the quantum fluctuations are ignored [17]. Mean-field approximations often require a lot less calculations than solving the original problem, so it may be used as a starting point to get an idea of how a solution may look like.

As a first step, a mean-field approximation is used to solve for the steady state of the given Lindblad equation, Eq. (6.1). Since the expectation value of an observable is given by the trace of the product of the observable and the density matrix, and since the trace is a linear operator; it commutes with the derivative, the expectation values of the spins may be calculated as

$$\frac{\mathrm{d}\langle\hat{S}_i\rangle}{\mathrm{d}t} = Tr(\hat{S}_i\dot{\rho}), \quad i = x, y, z. \tag{6.8}$$

To reach a solvable system the ansatz $\langle\hat{S}_i\hat{S}_j\rangle = \langle\hat{S}_i\rangle\langle\hat{S}_j\rangle$, for any spin operators $\hat{S}_i$, and $\hat{S}_j$, $i, j = x, y, z, +, -$ is used. It is this factorisation which forms the mean-field approximation; as mentioned previously, the quantum fluctuations arising from non commuting operators are neglected in this approximation, but since the corrections scale as $\frac{1}{N}$ this should be a good approximation of the model in the limit $N \longrightarrow \infty$. The factorisation is applied after the spin operators are systematised in a *normal order*[8], which means that all $\hat{S}_+$ operators in each term are on the left of the $\hat{S}_-$ operators. Using the commutation relations $[\hat{S}_+, \hat{S}_-] = 2\hat{S}_z$, and $[\hat{S}_z, \hat{S}_\pm] = \pm\hat{S}_\pm$, it is always possible to put the operators on normal order form.

First the expectation values for $\frac{\mathrm{d}\langle\hat{S}_j\rangle}{\mathrm{d}t}$, $j = +, -, z$ are calculated. The solutions are then transformed to the requested observables through the relation $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$. The calculation results in a non-linear system that must be solved to find the equations of motion,

$$\begin{gathered}
\frac{\mathrm{d}\langle\hat{S}_x\rangle}{\mathrm{d}t} = 2\frac{\kappa}{s}\langle\hat{S}_x\rangle\langle\hat{S}_z\rangle \\
\frac{\mathrm{d}\langle\hat{S}_y\rangle}{\mathrm{d}t} = \langle\hat{S}_z\rangle\left(2\frac{\kappa}{s}\langle\hat{S}_y\rangle - \omega\right) \\
\frac{\mathrm{d}\langle\hat{S}_z\rangle}{\mathrm{d}t} = \omega\langle\hat{S}_y\rangle - 2\frac{\kappa}{s}\left(\langle\hat{S}_x\rangle^2 + \langle\hat{S}_y\rangle^2\right).
\end{gathered} \tag{6.9}$$

As the square of the collective angular momentum operator $\hat{S}^2$, is a conserved quantity, $\langle\hat{S}^2\rangle = \langle\hat{S}_x^2\rangle + \langle\hat{S}_y^2\rangle + \langle\hat{S}_z^2\rangle$, and if the number of particles is large, $N \longrightarrow \infty$, $\langle\hat{S}^2\rangle \approx s^2$. Using this, the steady states solutions are calculated;

$$\left(\langle\hat{S}_x\rangle, \langle\hat{S}_y\rangle, \langle\hat{S}_z\rangle\right) = s\left(\pm\sqrt{1 - \frac{4\kappa^2}{\omega^2}}, \frac{2\kappa}{\omega}, 0\right) \tag{6.10}$$

and

$$\left(\langle\hat{S}_x\rangle, \langle\hat{S}_y\rangle, \langle\hat{S}_z\rangle\right) = s\left(0, \frac{\omega}{2\kappa}, \pm\sqrt{1 - \frac{\omega^2}{4\kappa^2}}\right) \tag{6.11}$$

The solutions are plotted in Fig. 4.

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[8] This is motivated by the *coherent state ansatz* which is used in mean-field approximations [17].

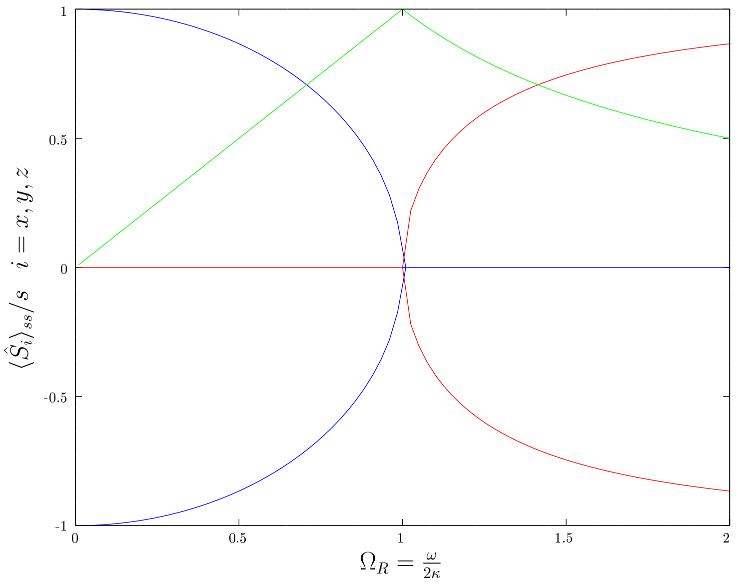

Figure 4: The expectation values $\langle \hat{S}_i \rangle_{ss}$, $i = x, y, z$, divided by the spin s for the steady state solution of the mean-field approximation as a function of the dimensionless quantity $\Omega_R = \frac{\omega}{2\kappa}$. The non-analyticity of the steady state is envisioned as the bifurcation at $\Omega_R = 1$. The colours correspond to each expectation value as: red: $i = x$, green: $i = y$, and blue: $i = z$.

It is of interest to understand the behaviour of the solutions in the neighbourhood of the fixed points, to explore the stability character of the solutions. If a fixed point is stable it will return or stay within a fixed radius of this point when displaced slightly away from the fixed point. An unstable fixed point will on the other hand diverge from the fixed point under such displacement, thus, one does not expect to find a system in such a solution [13].

To examine the stability, the system of equations is transformed to spherical coordinates (S, θ, φ), where S is the length of the total spin, θ the polar angle and φ the azimuthal angle. The total spin is constant so the system will in this form only consist of two equations which are

$$\dot{\theta} = 2\kappa \sin\theta - \omega \sin\varphi, \tag{6.12}$$

$$\dot{\varphi} = -\omega \frac{\cos\theta \cos\varphi}{\sin\theta}. \tag{6.13}$$

The fixed points for the above system are

$$(\theta,\varphi)=(\arcsin(\frac{\omega}{2\kappa}),\frac{\pi}{2}) \tag{6.14}$$

and

$$(\theta,\varphi)=(\arcsin(\frac{\omega}{2\kappa})+\frac{\pi}{2},\frac{\pi}{2}) \tag{6.15}$$

which are valid in the interval $\frac{\omega}{2\kappa}\in[0,1]$. $\varphi=-\frac{\pi}{2}$ is also a solution, but from the Cartesian system we know that y is positive. The other two steady state solutions are

$$(\theta,\varphi)=(\frac{\pi}{2},\arcsin(\frac{2\kappa}{\omega})), \tag{6.16}$$

$$(\theta,\varphi)=(\frac{\pi}{2},\arcsin(\frac{2\kappa}{\omega})+\frac{\pi}{2}) \tag{6.17}$$

which are valid for $\frac{\omega}{2\kappa}\geq 1$. To investigate the stability of the fixed points the system is linearised to first order which means that the *Jacobi matrix* (or *Jacobian* for short), $\hat{J}$ for the system is calculated,

$$\hat{J}=\begin{pmatrix} 2\kappa\cos\theta & -\omega\cos\varphi \\ \omega\cos\varphi\,(1+\cot^2\theta) & \omega\dfrac{\cos\theta\sin\varphi}{\sin\theta}\end{pmatrix}. \tag{6.18}$$

Next $\hat{J}$ is evaluated at each steady state solution, and the eigenvalues are calculated. For solutions Eq. (6.14) and Eq. (6.15) the Jacobians take the forms,

$$\hat{J}_{ss1}=\begin{pmatrix} 2\kappa\cos(\arcsin(\frac{\omega}{2\kappa})) & 0 \\ 0 & 2\kappa\cos(\arcsin(\frac{\omega}{2\kappa}))\end{pmatrix} \tag{6.19}$$

and

$$\hat{J}_{ss2}=\begin{pmatrix} -2\kappa\cos(\arcsin(\frac{\omega}{2\kappa})) & 0 \\ 0 & -2\kappa\cos(\arcsin(\frac{\omega}{2\kappa}))\end{pmatrix}. \tag{6.20}$$

Since $\cos(\arcsin(\frac{\omega}{2\kappa}))$ is positive in the first quadrant both eigenvalues for solution Eq. (6.14) are positive, hence this solution is unstable, but for

Eq. (6.15) both eigenvalues are negative, so this solution is stable, this solution corresponds to Eq. (6.11) for negative $\langle \hat{S}_z \rangle$. This makes sense when looking at the Lindblad equation (see Eq. (6.1)). Here the jump-operators are lowering operators, and when these are repeatedly applied to any state, the state will end up in the one with the spin pointing down in the z-direction. The Jacobians for the remaining steady state solutions are

$$\hat{J}_{ss3} = \begin{pmatrix} 0 & -\omega\cos(\arcsin(\frac{2\kappa}{\omega})) \\ \omega\cos(\arcsin(\frac{2\kappa}{\omega})) & 0 \end{pmatrix} \tag{6.21}$$

and

$$\hat{J}_{ss4} = \begin{pmatrix} 0 & \omega\cos(\arcsin(\frac{2\kappa}{\omega})) \\ -\omega\cos(\arcsin(\frac{2\kappa}{\omega})) & 0 \end{pmatrix}. \tag{6.22}$$

The eigenvalues for both matrices above are strictly imaginary, and since the system is linearised the stability of these fixed points is undecided, and it has to be investigated numerically. When checked numerically, it seems like both points are stable, but they behave in a peculiar way. When the fixed points are disturbed, the solutions move front and back within a radius away from the fixed point. However this radius grows as the initial disturbance is made larger. It is also strange that a physical system displays two stable solutions next to each other without an unstable solution sandwiched between them. This might be explained by the fact that we do have more solutions, if the complex solutions are included, but then, this should not be allowed since we are dealing with physical observables.

6.2 Exact analytical solution for the steady state

The exact steady state solution for Eq. (6.1) can be calculated analytically as shown by [14], and is

$$\rho_{ss} = \frac{1}{D} \sum_{m=0}^{2s} \sum_{n=0}^{2s} g^{*(-m)} g^{(-n)} \hat{S}_-^{(m)} \hat{S}_+^{(n)}, \tag{6.23}$$

valid for all spins s. Here $g = \frac{i\omega s}{\kappa}$, where ω and κ are the constants in the master equation, Eq. (6.1). $D = \mathrm{Tr}\rho_{ss}$ is the normalisation constant to ensure that $\mathrm{Tr}\rho_{ss} = 1$, and by calculating the trace using Dicke states, D is shown to be [16],

$$D = \sum_{m=0}^{2s} \frac{(2s+m+1)!(m!)^2}{(2s-m)!(2m+1)!} |g|^{-2m}. \qquad (6.24)$$

The density matrix may now be used to calculate any expectation values by using Eq. (2.11). In the following sections the steady state will be calculated numerically according to Eq. (6.23).

6.3 Numerical solution for the steady state

In this section the purity of the steady state as well as the expectation values obtained from the numerical evaluation of Eq. (6.23) are presented and analysed and a comparison with the mean-field solutions is made. Since it is not possible to do the numerical calculation in the limit of interest, $s \longrightarrow \infty$, all calculations are performed for a range of spins starting from low spins, of order $s = 10$, and ending at $s = 200$. The largest spin was chosen due to the rate of change of the expectation values as the spin was increased, together with the increase of the computational time. It was apparent from the computations that an increase from $s = 1$ to $s = 10$ resulted in a large change in the expectation values, for a low cost in computation time. But when increasing the spin from $s = 100$ to $s = 110$ the observation values changed very little in comparison with the large jump in computation time; this increase in computational time is due to the number of computations scaling as $(2s+1)^3$ for matrix multiplication.

The purity (see Eq. (2.18)) of the steady state as a function of the relative Rabi frequency, $\Omega_R = \frac{\omega}{\kappa}$ is plotted in Fig. 5, for spins $s = 10$, $s = 150$ and $s = 200$. The purity for Ω_R below the critical point is equal to, or very close to one, indicating that the state is pure. But as Ω_R grows beyond the critical point, the state becomes increasingly mixed. When the size of the spin is increased, the graph seems to take the form of a step function, with a non-analytical point at $\Omega_R = 1$. In the limit $s \longrightarrow \infty$ this is a critical point, Ω_c. In this case the state is pure when $\Omega_R < \Omega_c$ whilst it is maximally mixed when $\Omega_R > \Omega_c$. This might at a first glance seem counter intuitive, for small Ω_R the Lindblad terms dominate, and one might expect that the effects from the coupling to the environment would result in the state being mixed, whilst for a large Rabi frequency, the Hamiltonian should dominate and one might expect that the system in this case would be less mixed if not even pure, if we imagined that the system state is pure before the external field is switched on. However one must remember that it is the steady state solutions that are presented, which means that any information of the initial state is forgotten by the system. Nothing is said about the time scale of a physical system to reach a steady state. It may be extremely long, and the effects from the coupling to the environment might increase or decrease significantly during this time scale, resulting in the observed behaviour.

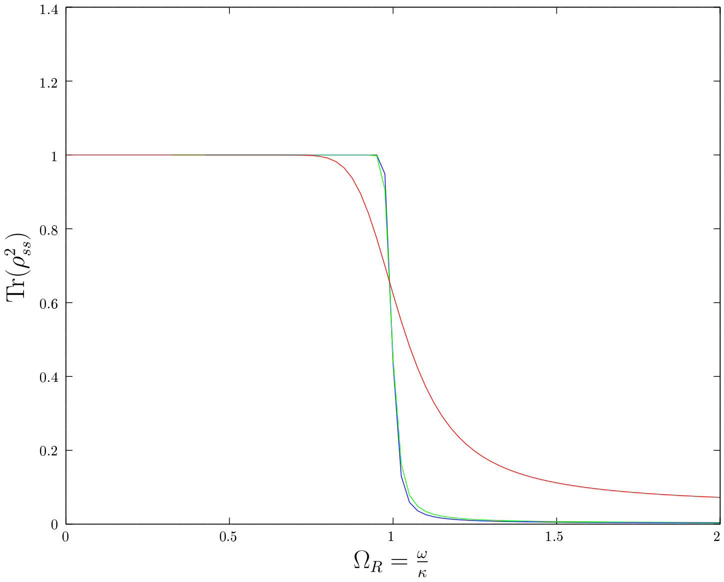

Figure 5: Purity of the steady state solution, $\mathrm{Tr}(\rho_{ss}^2)$, as a function of the dimensionless quantity $\Omega_R = \frac{\omega}{\kappa}$, for the different spins; red: $s = 10$, green: $s = 150$, and blue: $s = 200$. Note the small change between the blue and green curves, as discussed in the main text. It is evident that something drastic happens to the purity at the critical point; the state changes rapidly from pure into maximally mixed.

In Fig. 6 and Fig. 7, the expectation values $\langle \hat{S}_z \rangle$ and $\langle \hat{S}_y \rangle$ are plotted. In both cases it again seems that a non-analytic, critical, point is found at $\Omega_R = 1$ as the spin is increased towards infinity. The function $\langle \hat{S}_z \rangle$ is continuous and goes smoothly to zero at the critical point which hints that this represents a continuous phase transition, and from the observation of the purity of the system, the transition coincides with a state changing from a pure to a maximally mixed.

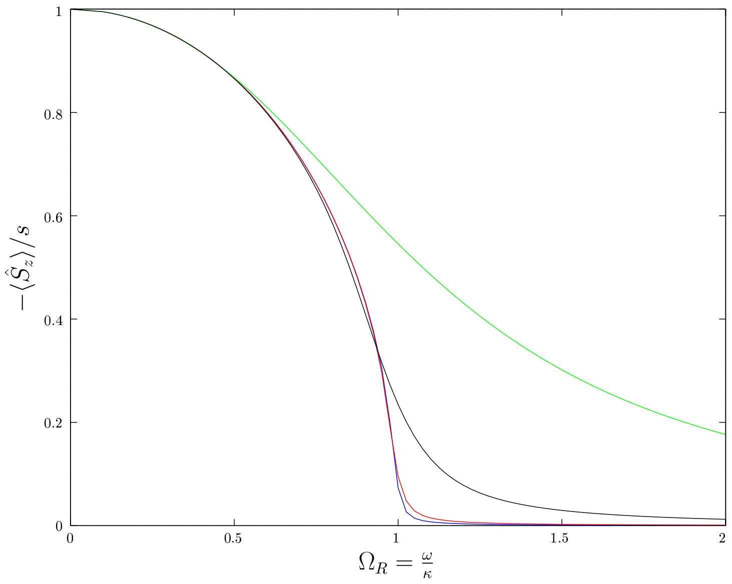

Figure 6: The expectation value, -$\langle\hat{S}_z\rangle$, divided by the spin, s, shown as a function of the dimensionless quantity $\Omega_R=\frac{\omega}{\kappa}$, for the different spins; green: $s=1$, black: $s=10$, red: $s=100$ and blue: $s=200$. The emergence of a non-analyticity is a typical signature of a continuos phase transition.

When comparing these results with the mean-field solution it can be seen that the mean-field approximation gives accurate predictions for the behaviour of $\langle\hat{S}_z\rangle$ and $\langle\hat{S}_y\rangle$ in the whole interval, when $s\longrightarrow\infty$. This is anticipated as mean-field approximations are expected to yield rather accurate results for a large system. Thus, the expectation value of $\hat{S}_y$ goes as Ω_R for $\Omega_R<\Omega_c$ and as $\frac{1}{\Omega_R}$ for $\Omega_R>\Omega_c$. The behaviour of $\langle\hat{S}_z\rangle$ follows that of the mean field solution for most of the range of Ω_R. But close to the critical point the solutions are not equal, which follows from the fact that the numerical solution is calculated for finite s. Although, the numerical solution moves closer and closer to the mean-field solution as the spin is increased, implying that they are equal as the spin becomes infinite. Since the stable mean field solution is given as $\langle\hat{S}_z\rangle_{MF}=-\sqrt{1-\Omega_R^2}$, it is expected that $\langle\hat{S}_z\rangle\propto|\lambda-\lambda_c|^{1/2}$; the analytic solution of the system would follow a power law with respect to a parameter $\lambda=\Omega_R^2$, with critical exponent $\nu=1/2$. The validity of this claim will be analysed in a later section. One may find it puzzling that $\langle\hat{S}_z\rangle$ seems to follow a typical scaling relation while $\langle\hat{S}_y\rangle$ does not. However, it should be remembered that the problem is two dimensional since the total spin is preserved, and hence $\langle\hat{S}_y\rangle$ is determined from the spin conservation constrain.

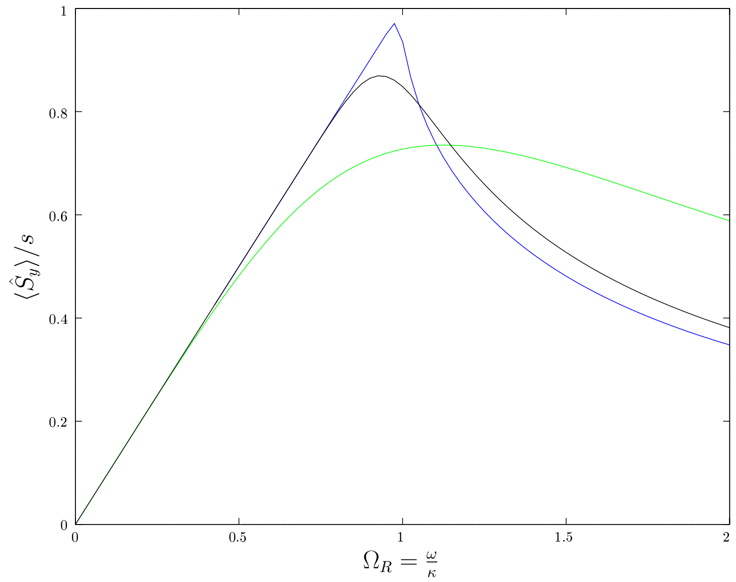

Figure 7: The expectation value, $\langle \hat{S}_y \rangle$, divided by the spin, s, as a function of the dimensionless quantity $\Omega_R = \frac{\omega}{\kappa}$, for the different spins; green: $s = 1$, black: $s = 10$ and blue: $s = 200$. Contrary to $\langle \hat{S}_z \rangle$, $\langle \hat{S}_y \rangle$ does not show the behaviour of an order parameter which is zero in one phase and non-zero in the other. The explanation for this qualitative difference between the two spin components results from the fact that the y-component is fixed by the conservation of total spin and by the equations of motion.

The expectation value, $\langle \hat{S}_x \rangle$ is constantly zero for all frequencies, and does not therefore agree with the mean-field solution when $\Omega_R > \Omega_c$, so in this region something happens which results in a breakdown of the mean-field approximation. To understand this, it is of interest to calculate the fluctuations $\langle \hat{S}_x^2 \rangle - \langle \hat{S}_x \rangle^2$, which are shown in Fig. 8. Since $\langle \hat{S}_x \rangle = 0$ this expectation value will from now on be simply be represented as $\langle \hat{S}_x^2 \rangle$. For large spins it seems that the fluctuations are close to zero for frequencies smaller than the critical point, to suddenly start growing at the critical point. When comparing the fluctuations of all three expectation values, as shown in Fig 9, they share this behaviour, and here it can also be seen that they all go towards $1/3$, which corresponds to the state with maximal uncertainty in each component of the spin. Since mean-field does not take quantum fluctuations into account one might think that these fluctuations are due to quantum uncertainties. On the other hand, quantum fluctuations are expected to be insignificantly small for large systems. When compared to the fluctuations of a pure state, where for example all spins point down in the $\hat{S}_x$ direction it can be seen that the quantum fluctuations for this state are of the order of the fluctuations for frequencies below the critical point in Fig. 8, and hence the large fluctuations for high frequencies should be given another explanation. These fluctuations arise instead due to uncertainties which occur as a result from the coupling to the environment, i.e. so called reservoir induced fluctuations which causes decoherence and thereby mixing of the system state.

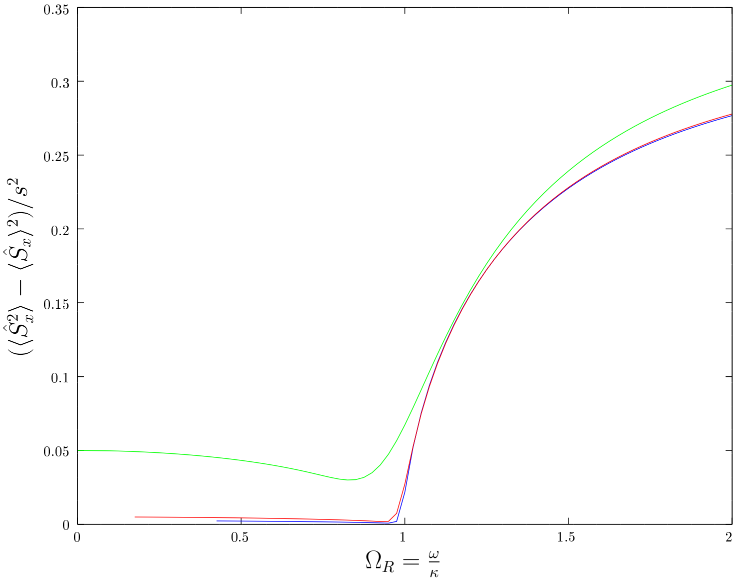

Figure 8: The expectation value, $\langle \hat{S}_x^2 \rangle - \langle \hat{S}_x \rangle^2$, divided by the spin squared, s^2, as a function of the dimensionless quantity $\Omega_R = \frac{\omega}{\kappa}$. The colours represent the different expectationvalues according to; green: $s = 10$, red: $s = 100$, and blue: $s = 200$. In the thermodynamic limit, the fluctuations in the region left of the critical point would vanish. Here, the fluctuations are of quantum nature, while to the right they are induced by the environment.

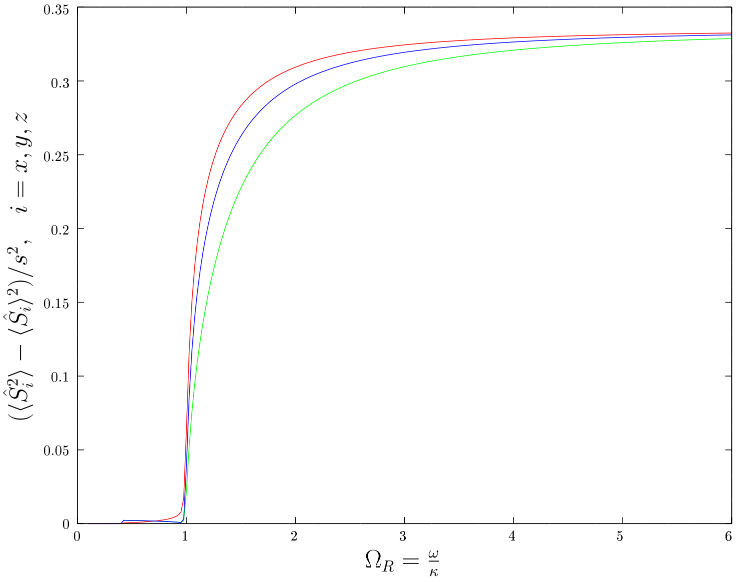

Figure 9: The expectation values, $(\langle\hat{S}_i^2\rangle - \langle\hat{S}_i\rangle^2)$, for $i = x, y, z$, for spin, $s = 200$ divided by s^2, as a function of the dimensionless quantity $\Omega_R = \frac{\omega}{\kappa}$. The colours represent the different expectationvalues according to; green: $i = x$, red: $i = z$, and blue: $i = y$. The asymptotic value for large Ω_R is $1/3$ and corresponds to a maximally mixed state.

Since the system is coupled to an environment, some information about the system is tied in the environment. When the environment is traced out, an uncertainty emerges, the more information that was shared, the higher the uncertainty. The idea that the fluctuations are due to effects from the coupling may also explain Fig. 5, the purity of the system. In the region to the right of the critical point, the state is maximally mixed, and the fluctuations are large; a large uncertainty may correspond to a stronger coupling, which would explain that the state is maximally mixed. However, in the region to the left of the critical point, the environment dominates, but the state is pure, so here it really must be an interplay between the environment and the system that gives this behaviour.

It is interesting that the mean-field solution is so different to the numerical solution with respect to the expectation value of $\hat{S}_x$. In addition, the mean-field solution gave peculiar results with respect to stability for these solutions, yielding two stable fixed points not separated by an unstable solution. This difference is most likely due to the fluctuations arising from the coupling, and how these appear/disappear in the mean-field solving process.

7 Critical exponents

Since the expectation value $\langle \hat{S}_z \rangle$ seems to approach a critical point at $\Omega_R = 1$ when $s \longrightarrow \infty$, with behaviour characteristic to that of a continuous phase transition, it is of interest whether a critical exponent can be subscribed to the behaviour of the expectation value in close vicinity of the critical point. When comparing the stable mean-field solution with the numerically calculated solution for $\langle \hat{S}_z \rangle$ it seems that they become equal in the limit of interest, which would suggest that a critical exponent of the mean-field solution and the numerical solution would be equal. The mean-field solution is described by the equation $\langle \hat{S}_z \rangle_{MF} = -|1 - \Omega_R^2|^{1/2}$, so if one chooses $\lambda = \Omega_R^2$ it may be expressed by a power law of the required form as $\langle \hat{S}_z \rangle_{MF} \propto |\lambda_c - \lambda|^{1/2}$, where λ_c is the critical point, and the critical exponent is 1/2. This is true for all $\lambda < \lambda_c$, not only in a close proximity from the critical point.

The evaluation whether the numerical solution approaches the same critical exponent as s is increased is performed by comparing the numerical solutions with the function

$$\langle \hat{S}_z \rangle_{MF} = -|1 - \Omega_R^2|^{1/2} \tag{7.1}$$

in the interval $\Omega_R \in [0.98, 1]$. An error between the numerical solutions, $\langle \hat{S}_z \rangle$ and $\langle \hat{S}_z \rangle_{MF}$ is estimated by first calculating the difference between the model and the numerical solutions in each point i as

$$\delta S_i = |\langle \hat{S}_z \rangle_{MF_i} - \langle \hat{S}_z \rangle_i|^2 \tag{7.2}$$

Then the uncertainty ΔS, is calculated as

$$\Delta S = \int_{0.98}^{1} \delta S \; \mathrm{d}\Omega_R. \tag{7.3}$$

The size of s is limited by the computation time, and is chosen for values between $s = 100$ and $s = 400$. The uncertainty is shown in Fig. 10, and from the figure it is clear that it decreases for increasing spin, especially when looking at the interval $\Omega_R \in [0.995, 1]$. It can therefore be suggested that the critical exponent for the system in the limit $s \longrightarrow \infty$ is $\frac{1}{2}$. The order parameter $\langle \hat{S}_z \rangle$ thus follows a power law with respect to λ, which suggests universality.

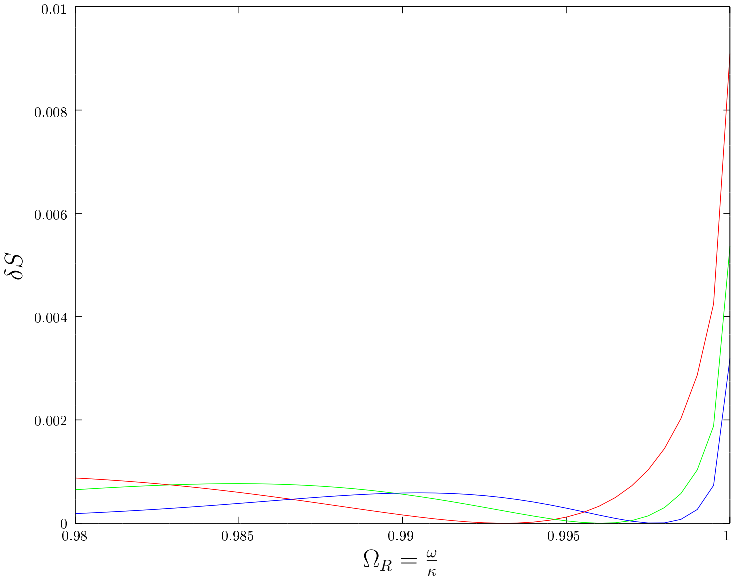

Figure 10: The plot shows the error, $\delta S = |\langle \hat{S}_z \rangle_{MF} - \langle \hat{S}_z \rangle|^2$, given as a function of the dimensionless quantity $\Omega_R = \frac{\omega}{\kappa}$, between the mean-field solution with critical exponent 1/2 and the numerical solutions for different spins, s, represented in the graph by the colours: red: $s = 100$, green: $s = 200$ and blue: $s = 400$. It is clear that the error is decreasing for increasing spin when the critical point is approached.

As previously mentioned, continuous phase transitions for systems in equilibrium commonly coincide with a spontaneous symmetry breaking. If the spin expectation values are good order parameters we see, however, that there is no symmetry breaking involved in varying λ. Nevertheless, it is interesting to ask whether there exists a companion state $\tilde{\rho}$, which permits expectation values symmetric to the ones calculated for ρ_{ss}, and which also solves the same Lindblad equation as ρ_{ss}. In other words, to search for a second steady state to the Lindblad equation. Such a state must be related to the first by the transformation

$$\tilde{\rho} : x \longrightarrow -x \quad y \longrightarrow y \quad z \longrightarrow -z. \tag{7.4}$$

This rotational transformation is performed by the unitary operator, $\hat{U} = e^{-i\pi\hat{S}_y}$, and the conjectured steady state would be $\tilde{\rho} = \hat{U}\rho\hat{U}^{-1}$. But it turns out that this state is not a simultaneous solution for the Lindblad equation describing our model, and it seems that one cannot talk about a symmetry nor a spontaneous symmetry breaking in relation to the phase transition. What we have found here, which is also a main conclusion of the thesis, is that this open quantum system obeys critical behaviour different to those common for systems in equilibrium. Even if we cannot say how general our results are, they open up for new mechanisms for phase transitions of non-equilibrium systems.

Another possible critical exponent of interest is the one for $\langle\hat{S}_x^2\rangle$, which exhibits the fluctuations due to the coupling between the system and its environment. In this case there is no mean-field solution to compare with, so instead another method is used. Since it is assumed that the expectation value can be written as

$$\langle\hat{S}_x^2\rangle = C|\lambda_c - \lambda|^{\nu}, \tag{7.5}$$

the exponent can be calculated by taking the logarithm of the above function,

$$f_1(\lambda) = \ln(\langle\hat{S}_x^2\rangle) = \ln C + \nu\ln|\lambda_c - \lambda|. \tag{7.6}$$

Again, encouraged from the previous result, $\lambda = \Omega_R^2$. The numerically calculated values of $\langle\hat{S}_x^2\rangle$ in the interval $\Omega_R \in [1, 1.1]$ for spins, $s = 50$ $s = 100$, $s = 200$ and $s = 400$ are then fitted to Eq. (7.6), through an un-weighted least square fit, from which values for the exponent ν can be extracted. These are of course different depending on the size of the spin and presented without uncertainties in Table. 2.

spin	50	100	200	400
C	0.1812	0.2051	0.2255	0.2398
ν	0.3745	0.4351	0.4776	0.5042

Table 2: The calculated values of the constants C and ν for spins, $s = 50, 100, 200$ and 400, from the un-weighted least square fit of $\ln(\langle\hat{S}_x^2\rangle)$ to a line, $f_1(\lambda) = \ln C + \nu\ln|\lambda_c - \lambda|$. The values are presented without errors with four significant numbers

It is not certain that the largest s gives the most correct fit in terms of the coefficients λ and C, because the curvature might change slightly when the spin is changed in a way that affects the fit, and the size of the two coefficients, even though their relative size stays the same. But since $s = 400$ is the best guess we have, the coefficient C_{400} for $s = 400$ is chosen as a fixed coefficient and the numerical solutions are fitted again, now to the to a line with

$$f_2(\lambda) = \ln C_{400} + \nu \ln|\lambda_c - \lambda|. \tag{7.7}$$

The value of the exponent ν is larger than in the first fit, and getting closer to 0.5. With two significant numbers, $\nu = 0.5$ is the same for spins $s = 200$ and $s = 400$. It would be interesting to see whether this is the case for higher spins, but without this information in hand $\nu = 0.5$ and $C = 0.24$ will have to do as the coefficients for our model.

spin	50	100	200	400
ν	0.4772	0.4922	0.5002	0.5042

Table 3: The calculated values of the constant ν for spins, $s = 50, 100, 200$ and 400, from the un-weighted least square fit of $\ln(\langle \hat{S}_x \rangle^2)$ to a line, $f_2(\lambda) = \ln C_{400} + \nu \ln|\lambda_c - \lambda|$. The values are presented without errors with four significant numbers. As is evident, the fit clearly suggest a critical exponent $\nu = 1/2$.

We have argued that the fluctuations represented by $\langle \hat{S}_x^2 \rangle$ are due to decoherence stemming from the coupling between the system and the environment, and as such it lacks a counterpart in a closed systems. This is why it is interesting to find that also this property, restricted to open systems, also seem to show scale invariance.

8 Entanglement

Entanglement is a concept of quantum mechanics which refers to correlations between two or more quantum systems, which are of such nature that they may not be explained within a classical theory [6]. For example, if a pure state system, AB, is divided into two subsystems A and B it is not implied that the states of these subsystems will also be pure, which is a contrast to classical systems [8]. If the states of the resulting subsystems are mixed, not all is known about them and this means that some information of system A is contained in system B and vice versa, which in return implies that there must be some correlation between states in system AB, i.e. the two subsystems are entangled [8]. In general, when the state of the full system is pure and possesses correlations between the two subsystems it is entangled [6]. But it becomes more complicated to draw similar conclusions of entanglement of a state which is mixed, since any mixed subsystems may then be mixed due to the mixedness inherent in the original state, and not due to correlations between the subsystems [6]. Such a mixed state of uncorrelated systems a and b may be expressed with a density operator

$$\rho_{ab} = \rho_a \otimes \rho_b. \tag{8.1}$$

A complete system composed by the mixture of the two systems is said to be *a correlated non-entangled* state and it has the form

$$\rho = \sum_{ij} P(a_i, b_j) \rho_a^i \otimes \rho_b^j. \tag{8.2}$$

On the other hand, if it is not possible to express a mixed state in this form, it is entangled [6]. However, the above logic goes only one way; there is no way to determine whether a general given mixed state is entangled or not. But there exists a sufficient condition for a mixed state to be entangled, which depends on the *partial transpose* of the density operator [6]. The partial transpose is defined as performing the transpose of only one of the systems in the tensor product in Eq. (8.2)

$$\rho^{PT} = \sum_{ij} P(a_i, b_j) \rho_a^i \otimes \rho_b^{j^T}. \tag{8.3}$$

Since the transpose of any density operator, here $\rho_b^{j^T}$, yields another density operator[9]; ρ^{PT}, is a density operator- a well defined physical state [6]. The partial transpose of a general mixed state operator may not yield a density operator; hence the mixed state may not be written in the form of Eq. (8.2), and must be entangled [6]. Since a density operator only can have positive eigenvalues, a sufficient condition for a state ρ to be entangled is that ρ^{PT}

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[9] The conditions that a density operator is Hermitian with positive eigenvalues and with a maximum trace equal to one, are all preserved when taking the transpose.

has negative eigenvalues, this is also a necessary condition for simple systems like qubits[10], but for higher dimensions no conclusions can be drawn about whether a state is entangled if it only has non negative eigenvalues [6]. A measurement of entanglement is the *Negativity*, for which all negative eigenvalues of the partial transpose of a density operator are summed, the higher negativity, the more entangled a state is [6]. This test of entanglement will be applied to the system considered in this thesis, where the system is divided into two equally sized subsystems. Another method of measuring entanglement is the *Concurrence* [18], it will be used as a measurement of entanglement between any pair of qubits of the complete system.

8.1 Negativity

In this section the negativity, $N(\lambda)$ is presented as a measure of the entanglement between two subsystems of the complete steady state solution. These two subsystems are equally large and calculated by taking the partial transpose of the density operator of the steady state. To get an expression for negativity, the matrix representation of the steady state is first divided into four blocks

$$\rho_{ss} = \begin{pmatrix} A & B \\ B^\dagger & C \end{pmatrix}. \tag{8.4}$$

Then the partial transpose is calculated by taking the transpose of each block

$$\rho^{PT} = \begin{pmatrix} A^T & B^T \\ B^{\dagger T} & C^T \end{pmatrix}. \tag{8.5}$$

The negativity, $N(\lambda)$ is the sum of all negative eigenvalues of ρ^{PT},

$$N(\lambda) = \sum_{i=1}^{2s} \frac{|\lambda_i| - \lambda_i}{2}. \tag{8.6}$$

The result is presented in Fig. (11) as a function of Ω_R. Since the system is large we cannot say anything about the entanglement when the negativity is zero, however when comparing the behaviour of the negativity with increasing

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[10] A qubit is a system which consists of only two states [6]

spin it is clear that the subsystems become increasingly entangled at the critical point, it almost looks like the negativity becomes a delta function at infinite spin. To understand how the negativity grows with respect to the size of the spin, the maximum value for the negativity is calculated for $s \in [0, 199.5]$ which shows that the negativity grows linearly with the spin, supporting the notion that the negativity will have a single peak at the critical point.

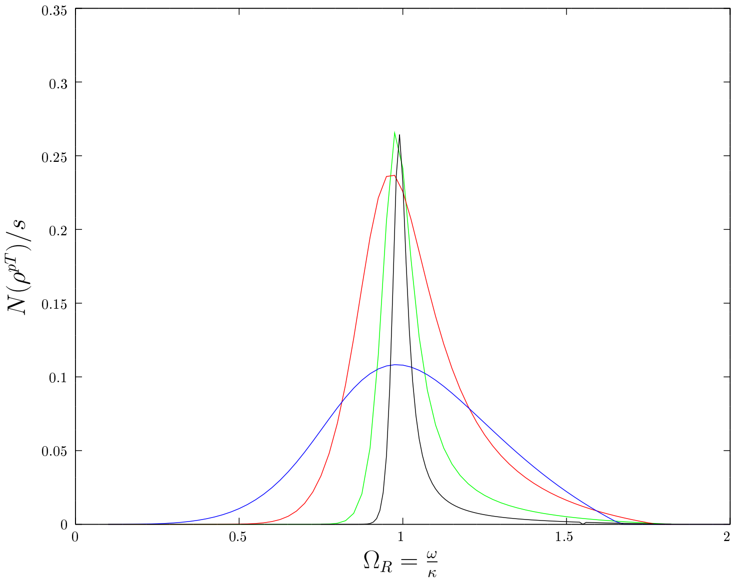

Figure 11: Plot of the negativity of the matrix ρ^{PT} which is the partial transpose of ρ_{ss}, divided with the spin, s, shown as a function of the dimensionless quantity $\Omega_R = \frac{\omega}{\kappa}$. The negativity is calculated for spins, $s = 3.5$ -blue, $s = 15.5$ -red, $s = 63.5$ -green and $s = 199.5$ -black. As is clear, the larger system (i.e. closer to the thermodynamic limit) the sharper peaked is the negativity around the critical point. It has also been verified numerically that the negativity at the critical point scales linear with the system size.

8.2 Concurrence

In this section the entanglement between a pair of atoms of the many atom system will be measured. The model considered is symmetrical in the sense that it does not matter which two particles are chosen. To get an expression for the steady state of a pair of qubits, the density matrix is first divided into

16 square blocks, A_{ij},

$$\rho_{ss} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{pmatrix}. \tag{8.7}$$

The trace of each block is the calculated to yield a density matrix for the steady state of two qubits

$$\rho_{ss}^{(2)} = \begin{pmatrix} \mathrm{Tr}(A_{11}) & \mathrm{Tr}(A_{12}) & \mathrm{Tr}(A_{13}) & \mathrm{Tr}(A_{14}) \\ \mathrm{Tr}(A_{21}) & \mathrm{Tr}(A_{22}) & \mathrm{Tr}(A_{23}) & \mathrm{Tr}(A_{24}) \\ \mathrm{Tr}(A_{31}) & \mathrm{Tr}(A_{32}) & \mathrm{Tr}(A_{33}) & \mathrm{Tr}(A_{34}) \\ \mathrm{Tr}(A_{41}) & \mathrm{Tr}(A_{42}) & \mathrm{Tr}(A_{43}) & \mathrm{Tr}(A_{44}) \end{pmatrix}. \tag{8.8}$$

The method now used, concurrence, is calculated according to a procedure, as explained in [18] and [19]. First the spin-flip transformation is introduced for a single qubit as

$$\rho \longrightarrow \bar{\rho} = \hat{\sigma}_y \rho^* \hat{\sigma}_y \tag{8.9}$$

where $\hat{\sigma}_y$ is the Pauli spin operator and ρ^* is the conjugate of ρ. The spin flip for two cubits is thus

$$\bar{\rho} = \hat{\sigma}_y \otimes \hat{\sigma}_y \rho^* \hat{\sigma}_y \otimes \hat{\sigma}_y, \tag{8.10}$$

from which an operator $\hat{g}$ is defined as

$$\hat{g} = \rho\,\bar{\rho}. \tag{8.11}$$

$\hat{g}$ has only positive eigenvalues and it is from these the concurrence, $C(\rho)$ is defined as

$$C(\rho) = \mathrm{Max}(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4). \tag{8.12}$$

λ_i, $i = 1, 2, 3, 4$ are the square roots of the eigenvalues of $\hat{g}$ in decreasing order, and $C(\rho)$ may only take values between zero and one. A zero concurrence corresponds to zero entanglement and the higher the concurrence, the more entangled are the two qubits forming the subsystem.

When the concurrence is calculated for increasing spin it can be seen in Fig. 12, that the maximum peaks closer and closer to the critical point and that the width decreases. Concurrence is not a multi-particle entanglement measure for the whole system but from the result it can be seen that entanglement between pairs of atoms exists in the system, especially around the critical point.

Both the negativity and concurrence show that entanglement exists between particles within the system, so also in the critical point, when $s \longrightarrow \infty$. This is interesting because the system is expected to behave classically in this limit, but still entanglement, a wholly quantum mechanical phenomena, is observed. These observations again demonstrate that our open model behaves differently compared to closed models. For a closed system it is also found that the entanglement diverges at the critical point, but in a power-law manner, i.e. one can assign critical exponents also for the behaviour of the entanglement in the vicinity of the critical point [20].

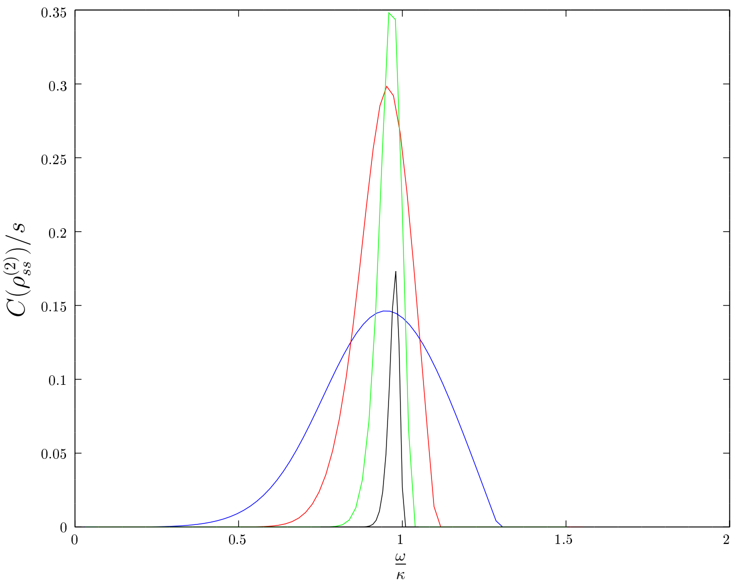

Figure 12: Plot of two particle concurrence, $C(\rho_{ss}^{(2)})$ divided by the spin, s, as a measure of entanglement, shown here as a function of the dimensionless quantity $\frac{\omega}{\kappa}$. The concurrence is calculated for spins, $s = 3.5$-blue, $s = 15.5$-red, $s = 63.5$-green $s = 203.5$-black. The concurrence seems to vanish everywhere apart from the critical point when the thermodynamic limit is taken, like the negativity displayed in Fig. 11.

9 Summary and conclusionary remarks

The aim of this thesis was to explore the critical behaviour of an open quantum system, by looking at a model which has an analytic solution for the steady state in the form of an infinite sum. The system consists of a collective large spin, comprised of N two level atoms connected to an external classical field. Systems in equilibrium are well understood when it comes to phase transitions and universality, in contrast to open quantum systems. But an advancement in the creation and control of open quantum systems in a lab environment opens up an interest to also study the critical behaviour of these kind of systems, and to explore similarities and differences between systems in and out of equilibrium.

The results demonstrate that the system undergoes a continuous phase transition, and that the transition displays universality; critical exponents for the expectation values $\langle \hat{S}_z \rangle$ and $\langle \hat{S}_x^2 \rangle$ are found. However, the system does not undergo a spontaneous symmetry breaking. This is a difference from systems in equilibrium, and it would be of interest to understand if this is a common feature in open quantum systems, or whether it is a feature of this particular model. The entanglement for the system is also measured, by looking at the negativity, and the concurrence. Since no method exists to measure the entanglement of a mixed state of general dimension, we cannot draw general conclusions of the entanglement of the whole system. But the results show that entanglement exists in the system, and does not disappear in the limit when s is large, where the entanglement peaks at the critical point for both methods. This is also interesting, since we expect the system to behave classically in this limit.

The resulting fluctuations measured seem to be to large to be quantum fluctuations and are expected to arise from the coupling with the bath. Since the mean-field results differ quite dramatically from the numerical ones with respect to the expectation value of $\langle \hat{S}_x \rangle$ it would be important to ask how these fluctuations are contained within the mean-field solution, and if/how they are the reason for the different results between the two solutions. A possible solution for this could be to replace factors of the form $\langle \hat{S}_i \rangle \langle \hat{S}_j \rangle$, $i, j = x, y, z$ in the mean-field equations, Eq.(6.9) with the calculated time derivatives of each product,

$$\frac{\mathrm{d}\langle \hat{S}_i \hat{S}_j \rangle}{\mathrm{d}t} = \mathrm{Tr}(\dot{\rho} \hat{S}_i \hat{S}_j). \tag{9.1}$$

This would yield products of more than two factors in each expectation value, but if this new system with more equations could be solved, it might give a result more consistent with the numerical solution as well as giving some insight into the behaviour of the fluctuations and how they are contained/discarded in the current mean-field solution.

The model that is considered in this thesis is relatively simple to solve since an analytic solution exists. But even so, it gave some interesting results on the criticality of an open quantum system, and exhibited differences in behaviour to the more well established results for systems in equilibrium. It would be of interest to next look at a more complex model with a more physical significance, and examine whether the same kind of critical behaviour emerges as was found here, to start to build up an understanding of open quantum systems in general.

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