Superradiant Effects in a Quantum Otto Cycle operated with Collective-Spin Models as a Working Fluid

Master's Thesis

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Abstract

Quantum heat engines operate with quantum matter as a working substance in thermodynamical cycles. The theoretical framework for their description is known as quantum thermodynamics, i.e. an intersection of two independent theories: quantum mechanics and thermodynamics. In recent years, superradiant effects have been discovered in different quantum heat machines. One of them is a quantum Otto cycle which uses a non-interacting collective-spin system, that dissipates coherently during the thermal strokes, leading to a superradiant boost in power. This effect in the collectivespin model is numerically studied. The same effect is studied for a quantum Otto cycle with an interacting collective-spin system which is modelled by taking the square of the responsible collectivespin operator. A master equation of Lindbladian type is derived with the Born-Markov and secular approximations, and used to operate the quantum Otto cycle with it. Hereby, a stronger superradiant effect is observed, as the typical quadratic scaling of power with the size of the system is evident even for lower temperatures. It is shown that the non-interacting collective-spin model is in most cases favourable in terms of power output, however there are settings, for which the interacting collectivespin model can outperform the non-interacting one. These settings can be achieved only by a fine tuning of all involved parameters. The validity range of the derived Linbladian master equation is also investigated for varying size of the system. It was shown that there is no violation of the assumptions as long as the working fluid's size and the temperatures of the heat baths are sufficiently small.



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1 Introduction

The field of quantum thermodynamics has become an active area of research in the last two decades, see [1] and references therein. A big aspect of it are investigations of quantum heat machines, which use quantum matter as a working substance in a quantum-thermodynamical cycle, since they serve as insightful model systems to study the relations between thermodynamics and quantum mechanics [2–4]. In 1959 Scovil and Schulz-DuBois were the first to link the efficiency of a three-level maser, which can be considered as the first quantum heat machine, to the Carnot efficiency [5]. Since then numerous models of this kind have been studied, e.g. the quantum Carnot cycle [6–8], the quantum Otto cycle [9–12], the quantum Stirling cycle [13, 14], and quantum refrigerators [15–18].

As for experimental evidence, there has recently been some progress in that regard [19–22]. For example, Roßnagel et al. [19] realized a single-atom heat engine in 2016, and Maslennikov et al. [21] were able to build a quantum absorption refrigerator using trapped Ytterbium ions. Despite of these first successes, an implementation of a heat machine fully operating in the quantum regime still remains a challenge.

Quantum heat machines have been discovered which exhibit superradiant effects [23–25]. One model consists of the quantum Otto cycle with coherent dissipation during the thermal strokes, which was described by Kloc, Cejnar, and Schaller in 2019 [26]. They have shown that this quantum heat engine exhibits a superradiant scaling in power, which required one of the two heat baths to be of relatively high temperature. In their conclusions Kloc, Cejnar, and Schaller proposed a model Hamiltonian of the type $H \propto J_z^2$ as the working fluid to be able to observe the superradiant scaling even for small temperatures. The goal of this work is to check this hypothesis. In order to do so, a detailed microscopic derivation of a Lindblad master equation for a general system coupled to an environment is presented in Section 2. This section follows closely Breuer and Petruccione [27], as well as Lidar [28] and serves to give a thourough understanding about this type of master equation. In Section 3 a short introduction to the quantum Otto cycle is given. Afterwards, following Kloc, Cejnar, and Schaller [26], a non-interacting collective-spin model is used as a working fluid for the quantum Otto cycle and a superradiant effect in power is investigated. In Section 4 an interacting collective-spin model is employed as a new working fluid of the proposed type for the heat machine, where the same properties as in the previous section are studied. A comparison with respect to power between these two models is given in Section 5. A discussion is presented in Section 6, and final conclusions are drawn in Section 7. Some additional information about superradiance and quantum relative entropy can be found in the Appendix.

Throughout the whole thesis, natural units have been used, i.e. $\hbar = k_{\rm B} = 1$. All numerical calculations have been carried out in Python 3.8. Additionally, for the non-interacting collective-spin model the package QuTiP 4.4.1 has been used which can be downloaded at http://qutip.org/download.html.

2 Microscopic Derivation of the Lindblad Master Equation for an Open Quantum System

There is a phenomenological derivation for a Lindblad master equation, which involves quantum dynamical semigroups [27], but a microscopic one is presented here. Later, there is a need to derive such a master equation for an interacting collective-spin model. Hence, it is reasonable to understand a derivation out of a microscopic perspective.

This whole section is, if not mentioned otherwise, entirely based on Breuer and Petruccione [27], and Lidar [28].

Consider a Hamiltonian $H(t) = H_{\rm S} + H_{\rm B} + H_{\rm I}$, where $H_{\rm S}$ is a system Hamiltonian, $H_{\rm B}$ is a Hamiltonian for the environment (e.g. a heat bath), and $H_{\rm I} = g \sum_n A_n \otimes B_n$ describes the interaction between the system and the environment (see Figure 2.1). Here, g is a coupling parameter, A_n are system operators and B_n are environment operators. Later there will be a Marov approximation applied which is based on a weak coupling of the system to its environment. Thus, any terms of order g^3 or higher are neglected. The system and bath operators are assumed to commute, i.e. $[A_n, B_{n'}] = 0$ for all n, n'. Because these operators commute, the corresponding Hilbert space of this whole quantum system can be written as a Kronecker product of the Hilbert spaces of the system and the environment respectively, i.e.

$$\mathscr{H} = \mathscr{H}_{S} \otimes \mathscr{H}_{B}. \tag{2.1}$$



Figure 2.1: Visualization of the total Hamiltonian H(t). $H_{\rm S}$ represents an arbitrary system coupled to an environment, given by $H_{\rm B}$. The interaction between the two is described by $H_{\rm I}$.

In order to describe the evolution of an open quantum system, it is necessary to use the density matrix formalism. Starting with the von Neumann equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -i\left[H(t),\rho(t)\right] = -i\left[H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{I}},\rho(t)\right],\tag{2.2}$$

one first makes a transition to the interaction picture. Let $H(t) = H_0 + H_I$, where $H_0 = H_S + H_B$. The time evolution of the density matrix in the interaction picture is then given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}(t) = -i\left[\hat{H}(t), \hat{\rho}(t)\right],\tag{2.3}$$

where

$$\hat{\rho}(t) = e^{iH_0 t} \rho e^{-iH_0 t}, \tag{2.4}$$

$$\hat{H}(t) = e^{iH_0 t} H_{\rm I} e^{-iH_0 t}.$$
(2.5)

As shown below, the interaction Hamiltonian can be expressed as

$$\hat{H}(t) = g \sum_{n} \hat{A}_{n} \otimes \hat{B}_{n}, \qquad (2.6)$$

with $\hat{A}_n = e^{iH_{\rm S}t}A_n e^{-iH_{\rm S}t}$ and $\hat{B}_n = e^{iH_{\rm B}t}B_n e^{-iH_{\rm B}t}$.

Claim: The interaction-picture Hamiltonian is given by $\hat{H}(t) = g \sum_{n} \hat{A}_{n} \otimes \hat{B}_{n}$.

Proof:

Note that for simplicity some Kronecker products were omitted in the free Hamiltonian H_0 . Writing them out yields

$$H_0 = H_{\rm S} \otimes \mathbb{1}_{\rm B} + \mathbb{1}_{\rm S} \otimes H_{\rm B}.$$

Plugging this in the expression in equation (2.5) gives

$$\hat{H}(t) = e^{i(H_{\rm S} \otimes \mathbb{1}_{\rm B} + \mathbb{1}_{\rm S} \otimes H_{\rm B})t} H_{\rm I} e^{-i(H_{\rm S} \otimes \mathbb{1}_{\rm B} + \mathbb{1}_{\rm S} \otimes H_{\rm B})t}.$$

Using the Kronecker sum [29], this can be rewritten to

$$\hat{H}(t) = \left(e^{iH_{\rm S}t} \otimes e^{iH_{\rm B}t}\right) H_{\rm I} \left(e^{-iH_{\rm S}t} \otimes e^{-iH_{\rm B}t}\right).$$

Using the definition of $H_{\rm I}$ results in

$$\hat{H}(t) = \left(e^{iH_{\mathrm{S}}t} \otimes e^{iH_{\mathrm{B}}t}\right) \left(g\sum_{n} A_{n} \otimes B_{n}\right) \left(e^{-iH_{\mathrm{S}}t} \otimes e^{-iH_{\mathrm{B}}t}\right)$$

$$= g\sum_{n} \left(e^{iH_{\mathrm{S}}t} \otimes e^{iH_{\mathrm{B}}t}\right) \left(A_{n} \otimes B_{n}\right) \left(e^{-iH_{\mathrm{S}}t} \otimes e^{-iH_{\mathrm{B}}t}\right)$$

$$= g\sum_{n} \left(e^{iH_{\mathrm{S}}t} \otimes e^{iH_{\mathrm{B}}t}\right) \left(A_{n}e^{-iH_{\mathrm{S}}t} \otimes B_{n}e^{-iH_{\mathrm{B}}t}\right)$$

$$= g\sum_{n} \left(e^{iH_{\mathrm{S}}t} A_{n}e^{-iH_{\mathrm{S}}t}\right) \otimes \left(e^{iH_{\mathrm{B}}t} B_{n}e^{-iH_{\mathrm{B}}t}\right)$$

$$= g\sum_{n} \hat{A}_{n} \otimes \hat{B}_{n}$$

with $\hat{A}_n := e^{iH_{\mathrm{S}}t}A_n e^{-iH_{\mathrm{S}}t}$ and $\hat{B}_n := e^{iH_{\mathrm{B}}t}B_n e^{-iH_{\mathrm{B}}t}$.

Equation (2.3) can be rewritten in an integral form as

$$\hat{\rho}(t) = \hat{\rho}(t_0) - i \int_{t_0}^t dt' \left[\hat{H}(t'), \hat{\rho}(t') \right].$$
(2.7)

Because t_0 represents the point in time, where the whole quantum system starts to evolve in time, $t_0 = 0$ can be chosen. Plugging this integral form back in equation (2.3) yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}(t) = -i \left[\hat{H}(t), \hat{\rho}(0) - i \int_{0}^{t} \mathrm{d}t' \left[\hat{H}(t'), \hat{\rho}(t')\right]\right]
= -i \left[\hat{H}(t), \hat{\rho}(0)\right] - \int_{0}^{t} \mathrm{d}t' \left[\hat{H}(t), \left[\hat{H}(t'), \hat{\rho}(t')\right]\right],$$
(2.8)

which is an integro-differential equation. Equation (2.8) is exact, but highly non-linear. To be able to solve it, some approximations are necessary.

2.1 Born Approximation

Let the environment be a heat bath. If it is much larger than the system, then all backactions on the bath caused by small non-trivial evolutions of the system can be neglected. This means that the state of the composite system can be approximated as

$$\hat{\rho}(t) \approx \hat{\rho}_{\rm S}(t) \otimes \hat{\rho}_{\rm B}, \tag{2.9}$$

where $\hat{\rho}_{\rm B}$ is a stationary bath state. Plugging equation (2.9) in equation (2.8) gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{\rho}_{\mathrm{S}}(t)\otimes\hat{\rho}_{\mathrm{B}}\right) = -i\left[\hat{H}(t),\hat{\rho}_{\mathrm{S}}(0)\otimes\hat{\rho}_{\mathrm{B}}\right] - \int_{0}^{t}\mathrm{d}t'\left[\hat{H}(t),\left[\hat{H}(t'),\hat{\rho}_{\mathrm{S}}(t')\otimes\hat{\rho}_{\mathrm{B}}\right]\right].$$
(2.10)

The degrees of freedom of the bath can be traced out by taking the partial trace. The left-hand side of the equation results in

$$\begin{aligned} \operatorname{Tr}_{\mathrm{B}}\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{\rho}_{\mathrm{S}}(t)\otimes\hat{\rho}_{\mathrm{B}}\right)\right] &= \operatorname{Tr}_{\mathrm{B}}\left[\left(\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t)\right)\otimes\hat{\rho}_{\mathrm{B}} + \hat{\rho}_{\mathrm{S}}(t)\otimes\left(\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{B}}\right)\right] \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t)\cdot\operatorname{Tr}\left(\hat{\rho}_{\mathrm{B}}\right) \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t), \end{aligned} \tag{2.11}$$

where the assumption that $\hat{\rho}_{\rm B}$ is a steady state has been used.

The right-hand side of equation (2.10) yields

$$\operatorname{Tr}_{\mathcal{B}}\left[-i\left[\hat{H}(t), \hat{\rho}_{\mathcal{S}}(0) \otimes \hat{\rho}_{\mathcal{B}}\right] - \int_{0}^{t} \mathrm{d}t'\left[\hat{H}(t), \left[\hat{H}(t'), \hat{\rho}_{\mathcal{S}}(t') \otimes \hat{\rho}_{\mathcal{B}}\right]\right]\right] = \\ \underbrace{-i\operatorname{Tr}_{\mathcal{B}}\left[\left[\hat{H}(t), \hat{\rho}_{\mathcal{S}}(0) \otimes \hat{\rho}_{\mathcal{B}}\right]\right]}_{(*)} - \int_{0}^{t} \mathrm{d}t'\operatorname{Tr}_{\mathcal{B}}\left[\left[\hat{H}(t), \left[\hat{H}(t'), \hat{\rho}_{\mathcal{S}}(t') \otimes \hat{\rho}_{\mathcal{B}}\right]\right]\right].$$
(2.12)

The term denoted with (*) can be evaluated by employing the expression of the interaction-picture Hamiltonian (2.6).

$$(*) = -i \operatorname{Tr}_{B} \left[\left[g \sum_{n} \hat{A}_{n} \otimes \hat{B}_{n}, \hat{\rho}_{S}(0) \otimes \hat{\rho}_{B} \right] \right]$$

$$= -ig \sum_{n} \operatorname{Tr}_{B} \left[\left(\hat{A}_{n} \otimes \hat{B}_{n} \right) \left(\hat{\rho}_{S}(0) \otimes \hat{\rho}_{B} \right) - \left(\hat{\rho}_{S}(0) \otimes \hat{\rho}_{B} \right) \left(\hat{A}_{n} \otimes \hat{B}_{n} \right) \right]$$

$$= -ig \sum_{n} \operatorname{Tr}_{B} \left[\hat{A}_{n} \hat{\rho}_{S}(0) \otimes \hat{B}_{n} \hat{\rho}_{B} - \hat{\rho}_{S}(0) \hat{A}_{n} \otimes \hat{\rho}_{B} \hat{B}_{n} \right]$$

$$= -ig \sum_{n} \hat{A}_{n} \hat{\rho}_{S}(0) \operatorname{Tr} \left(\hat{B}_{n} \hat{\rho}_{B} \right) - \hat{\rho}_{S}(0) \hat{A}_{n} \underbrace{\operatorname{Tr} \left(\hat{\rho}_{B} \hat{B}_{n} \right)}_{= \operatorname{Tr} \left(\hat{B}_{n} \hat{\rho}_{B} \right)}$$

$$= -ig \sum_{n} \langle \hat{B}_{n} \rangle \left[\hat{A}_{n}, \hat{\rho}_{S}(0) \right], \qquad (2.13)$$

with $\langle \hat{B}_n \rangle := \text{Tr}\left(\hat{B}_n \hat{\rho}_{\text{B}}\right)$. With these calculations equation (2.10) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -ig\sum_{n} \langle \hat{B}_{n} \rangle \left[\hat{A}_{n}, \hat{\rho}_{\mathrm{S}}(0) \right] - \int_{0}^{t} \mathrm{d}t' \operatorname{Tr}_{\mathrm{B}} \left[\left[\hat{H}(t), \left[\hat{H}(t'), \hat{\rho}_{\mathrm{S}}(t') \otimes \hat{\rho}_{\mathrm{B}} \right] \right] \right].$$
(2.14)

The first term on the right-hand side is a sum of commutators that are proportional to the expectation values of the bath operators $\langle \hat{B}_n \rangle$. Because there exists a transformation that sets these to zero [30], this term vanishes and equation (2.14) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -\int_{0}^{t} \mathrm{d}t' \operatorname{Tr}_{\mathrm{B}}\left[\left[\hat{H}(t), \left[\hat{H}(t'), \hat{\rho}_{\mathrm{S}}(t') \otimes \hat{\rho}_{\mathrm{B}}\right]\right]\right].$$
(2.15)

Claim: There is a transformation $\hat{B}_n \longrightarrow \hat{B}'_n$, so that $\langle \hat{B}'_n \rangle = 0$.

Proof:

Let $\hat{B}_n = \sum_m \lambda_m |m\rangle \langle m|$ the spectral decomposition of \hat{B}_n and let $\hat{B}_d^{(n)} = \text{diag}\left(\hat{B}_n\right) = \sum_m \hat{B}_{mm}^{(n)} |m\rangle \langle m|$.

Note: For an arbitrary observable A and density matrix
$$\rho = \sum_{i} p_i |\Phi_i\rangle \langle \Phi_i|$$
, the expectation value is

$$\langle A \rangle = \operatorname{Tr} (A\rho) = \sum_{i} p_i \langle \Phi_i | A | \Phi_i \rangle.$$

Choose a transformation

$$\hat{B}_n \longrightarrow \hat{B}'_n = \hat{B}_n - \hat{B}_d^{(n)}$$

$$\Rightarrow \langle \hat{B}'_n \rangle = \langle \hat{B}_n - \hat{B}^{(n)}_d \rangle$$
$$= \sum_m \lambda_m \langle m | \hat{B}_n - \hat{B}^{(n)}_d | m \rangle = \sum_m \lambda_m \left(\langle m | \hat{B}_n | m \rangle - \langle m | \hat{B}^{(n)}_d | m \rangle \right)$$
$$= \sum_m \lambda_m \left(\langle m | \hat{B}_n | m \rangle - \langle m | \sum_k \hat{B}^{(n)}_{kk} | k \rangle \langle k | m \rangle \right)$$
$$= \sum_m \lambda_m \left(\langle m | \hat{B}_n | m \rangle - \langle m | \hat{B}^{(n)}_{mm} | m \rangle \right) = 0.$$

Note that with this transformation, the Hamiltonian $\hat{H}(t)$ is also transformed, but for simplicity, all corresponding primes are omitted.

Continuing with equation (2.15), the next step is to plug in equation (2.6) and evaluate the partial trace,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) &= -\int_{0}^{t} \mathrm{d}t' \operatorname{Tr}_{\mathrm{B}}\left[\left[g \sum_{n} \hat{A}_{n}(t) \otimes \hat{B}_{n}(t), \left[g \sum_{m} \hat{A}_{m}(t') \otimes \hat{B}_{m}(t'), \hat{\rho}_{\mathrm{S}}(t') \otimes \hat{\rho}_{\mathrm{B}} \right] \right] \right] \\ &= -g^{2} \sum_{n} \sum_{m} \int_{0}^{t} \mathrm{d}t' \operatorname{Tr}_{\mathrm{B}}\left[\hat{A}_{n}(t) \hat{A}_{m}(t') \hat{\rho}_{\mathrm{S}}(t') \otimes \hat{B}_{n}(t) \hat{B}_{m}(t') \hat{\rho}_{\mathrm{B}} - \hat{A}_{n}(t) \hat{\rho}_{\mathrm{S}}(t') \hat{A}_{m}(t') \right] \end{aligned}$$

$$\begin{split} &\otimes \hat{B}_{n}(t)\hat{\rho}_{B}\hat{B}_{m}(t') - \hat{A}_{m}(t')\hat{\rho}_{S}(t')\hat{A}_{n}(t) \otimes \hat{B}_{m}(t')\hat{\rho}_{B}\hat{B}_{n}(t) + \hat{\rho}_{S}(t')\hat{A}_{m}(t')\hat{A}_{n}(t) \\ &\otimes \hat{\rho}_{B}\hat{B}_{m}(t')\hat{B}_{n}(t) \bigg] \\ &= -g^{2}\sum_{n}\sum_{m}\int_{0}^{t} dt' \hat{A}_{n}(t)\hat{A}_{m}(t')\hat{\rho}_{S}(t')\text{Tr}\left(\hat{B}_{n}(t)\hat{B}_{m}(t')\hat{\rho}_{B}\right) - \hat{A}_{n}(t)\hat{\rho}_{S}(t')\hat{A}_{m}(t') \\ &\quad \cdot \text{Tr}\left(\hat{B}_{n}(t)\hat{\rho}_{B}\hat{B}_{m}(t')\right) - \hat{A}_{m}(t')\hat{\rho}_{S}(t')\hat{A}_{n}(t)\text{Tr}\left(\hat{B}_{m}(t')\hat{\rho}_{B}\hat{B}_{n}(t)\right) + \hat{\rho}_{S}(t')\hat{A}_{m}(t')\hat{A}_{n}(t) \\ &\quad \cdot \text{Tr}\left(\hat{\rho}_{B}\hat{B}_{m}(t')\hat{B}_{n}(t)\right). \end{split}$$

$$(2.16)$$

The traces can now be identified with two-time bath-correlation functions. Thus, it is reasonable to write

$$\operatorname{Tr}\left(\hat{B}_{m}(t')\hat{\rho}_{B}\hat{B}_{n}(t)\right) = \operatorname{Tr}\left(\hat{B}_{n}(t)\hat{B}_{m}(t')\hat{\rho}_{B}\right) =: \langle \hat{B}_{n}(t)\hat{B}_{m}(t')\rangle, \qquad (2.17)$$

$$\operatorname{Tr}\left(\hat{B}_{n}(t)\hat{a}_{B}\hat{B}_{n}(t')\right) = \operatorname{Tr}\left(\hat{a}_{n}\hat{B}_{n}(t')\hat{B}_{n}(t)\right) = \operatorname{Tr}\left(\hat{B}_{n}(t')\hat{B}_{n}(t)\hat{a}_{n}\right) =: \langle \hat{B}_{n}(t')\hat{B}_{n}(t')\rangle, \qquad (2.18)$$

$$\operatorname{Tr}\left(\hat{B}_{n}(t)\hat{\rho}_{\mathrm{B}}\hat{B}_{m}(t')\right) = \operatorname{Tr}\left(\hat{\rho}_{\mathrm{B}}\hat{B}_{m}(t')\hat{B}_{n}(t)\right) = \operatorname{Tr}\left(\hat{B}_{m}(t')\hat{B}_{n}(t)\hat{\rho}_{\mathrm{B}}\right) =: \langle\hat{B}_{m}(t')\hat{B}_{n}(t)\rangle.$$
(2.18)

Hence, one obtains

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -g^{2}\sum_{n}\sum_{m}\int_{0}^{t}\mathrm{d}t' \left[\hat{A}_{n}(t),\hat{A}_{m}(t')\hat{\rho}_{\mathrm{S}}(t')\right]\langle\hat{B}_{n}(t)\hat{B}_{m}(t')\rangle + \left[\hat{\rho}_{\mathrm{S}}(t')\hat{A}_{m}(t'),\hat{A}_{n}(t)\right]\langle\hat{B}_{m}(t')\hat{B}_{n}(t)\rangle.$$
(2.19)

Claim: The two-time correlation functions obey $\langle \hat{B}_n(t)\hat{B}_m(t')\rangle = \langle \hat{B}_n(t-t')\hat{B}_m(0)\rangle$.

Proof:

Remember that the operators in $\langle \hat{B}_n(t)\hat{B}_m(t')\rangle$ are in the interaction picture. This gives

$$\langle \hat{B}_n(t)\hat{B}_m(t')\rangle = \operatorname{Tr}\left(\hat{B}_n(t)\hat{B}_m(t')\hat{\rho}_{\mathrm{B}}\right)$$

$$= \operatorname{Tr}\left(e^{iH_{\mathrm{B}}t}B_n e^{-iH_{\mathrm{B}}t}e^{iH_{\mathrm{B}}t'}B_m e^{-iH_{\mathrm{B}}t'}\hat{\rho}_{\mathrm{B}}\right)$$

$$= \operatorname{Tr}\left(e^{iH_{\mathrm{B}}(t-t')}B_n e^{-iH_{\mathrm{B}}(t-t')}B_m\hat{\rho}_{\mathrm{B}}\right)$$

$$= \operatorname{Tr}\left(\hat{B}_n(t-t')\hat{B}_m(0)\hat{\rho}_{\mathrm{B}}\right)$$

$$= \langle \hat{B}_n(t-t')\hat{B}_m(0)\rangle$$

Defining $\langle \hat{B}_n(t-t')\hat{B}_m(0)\rangle =: \bar{B}_{nm}(t-t',0)$, and using

$$\begin{bmatrix} \hat{\rho}_{\rm S}(t')\hat{A}_m(t'), \hat{A}_n(t) \end{bmatrix} = \hat{\rho}_{\rm S}(t')\hat{A}_m(t')\hat{A}_n(t) - \hat{A}_n(t)\hat{\rho}_{\rm S}(t')\hat{A}_m(t') = \left(\hat{A}_n(t)\hat{A}_m(t')\hat{\rho}_{\rm S}(t') - \hat{A}_m(t')\hat{\rho}_{\rm S}(t')\hat{A}_n(t)\right)^{\dagger} = \left[\hat{A}_n(t), \hat{A}_m(t')\hat{\rho}_{\rm S}(t')\right]^{\dagger}, \quad (2.20)$$

leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -g^{2}\sum_{n}\sum_{m}\int_{0}^{t}\mathrm{d}t' \left[\hat{A}_{n}(t), \hat{A}_{m}(t')\hat{\rho}_{\mathrm{S}}(t')\right]\bar{B}_{nm}(t-t',0) + \left[\hat{A}_{n}(t), \hat{A}_{m}(t')\hat{\rho}_{\mathrm{S}}(t')\right]^{\dagger}\bar{B}_{mn}(t'-t,0).$$
(2.21)

Claim: The bath-correlation function fulfills $\bar{B}_{mn}(t'-t,0) = \bar{B}_{nm}^*(t-t',0)$.

Proof:

$$\begin{split} \bar{B}_{mn}(t'-t,0) &= \bar{B}_{mn}(-(t-t'),0) = \operatorname{Tr}\left(e^{-iH_{\mathrm{B}}(t-t')}B_{m}e^{iH_{\mathrm{B}}(t-t')}B_{n}\hat{\rho}_{\mathrm{B}}\right) \\ &= \operatorname{Tr}\left(\hat{\rho}_{\mathrm{B}}B_{m}e^{iH_{\mathrm{B}}(t-t')}B_{n}e^{-iH_{\mathrm{B}}(t-t')}\right) \\ &= \operatorname{Tr}\left(\left(e^{iH_{\mathrm{B}}(t-t')}B_{n}e^{-iH_{\mathrm{B}}(t-t')}B_{m}\hat{\rho}_{\mathrm{B}}\right)^{\dagger}\right) \\ &= \operatorname{Tr}\left(e^{iH_{\mathrm{B}}(t-t')}B_{n}e^{-iH_{\mathrm{B}}(t-t')}B_{m}\hat{\rho}_{\mathrm{B}}\right)^{\ast} \\ &= \bar{B}_{nm}^{\ast}(t-t',0). \end{split}$$

With this, equation (2.21) simplifies to

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -g^{2}\sum_{n}\sum_{m}\int_{0}^{t}\mathrm{d}t' \left[\hat{A}_{n}(t), \hat{A}_{m}(t')\hat{\rho}_{\mathrm{S}}(t')\right]\bar{B}_{nm}(t-t',0) + \mathrm{h.c.}.$$
(2.22)

Thanks to the Born approximation, the dynamics of the bath are now being captured solely by the bath-correlation functions. Making a change of variables by substituting $\tau := t - t'$, equation (2.22) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -g^{2}\sum_{n}\sum_{m}\int_{0}^{t}\mathrm{d}\tau \,\left[\hat{A}_{n}(t),\hat{A}_{m}(t-\tau)\hat{\rho}_{\mathrm{S}}(t-\tau)\right]\bar{B}_{nm}(\tau,0) + \mathrm{h.c..}$$
(2.23)

2.2 Markov Approximation

On the right-hand side of equation (2.23), the argument of $\hat{\rho}_{\rm S}$ is integrated over the interval [0, t]. Thus, the evolution of the system at times t is dependent on its whole history. This means that all effects have significant consequences later on. Therefore, equation (2.23) is time non-local. To get a time-local equation, where the state of the system depends on t, but not on its history, a Markov approximation is necessary.

Let the system be weakly coupled to the heat bath and all correlations within the bath are, compared to the relaxation time of the system, rapidly decaying with some characteristic time scale $\tau_{\rm B}$. Formally these assumptions can be written as

$$g \ll 1/\tau_{\rm B}$$
 and $t \gg \tau_{\rm B}$. (2.24)

These conditions lead to a 'short-memory' effect, i.e. the bath correlation function keeps track of events only within the time interval $[0, \tau_{\rm B}]$. Thus, $\hat{\rho}_{\rm S}(t - \tau)$ can be replaced with $\hat{\rho}_{\rm S}(t)$ and the upper integral limit of equation (2.23) can be expanded to infinity without changing the integrand. Hence, with the Markov approximation equation (2.23) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -g^2 \sum_{n} \sum_{m} \int_{0}^{\infty} \mathrm{d}\tau \left[\hat{A}_{n}(t), \hat{A}_{m}(t-\tau)\hat{\rho}_{\mathrm{S}}(t)\right] \bar{B}_{nm}(\tau, 0) + \mathrm{h.c.}.$$
(2.25)

In this form this equation is known as a Redfield master equation. Such equations are known to not ensure the positivity of $\hat{\rho}_{\rm S}(t)$ during its time evolution [30,31]. To avoid this problem, one uses a third approximation, known as the rotating wave approximation or secular approximation. This enables the equation to be written in Lindblad form, guaranteeing no violation of the defining properties of $\hat{\rho}_{\rm S}(t)$.

To be able to perform the secular approximation, one goes to the energy domain by decomposing $\hat{H}(t)$ into eigenoperators of $H_{\rm S}$.

Using the spectral decomposition of $H_{\rm S} = \sum_{a} \varepsilon_a |\varepsilon_a\rangle \langle \varepsilon_a|$ the operator $\hat{A}_n(t)$ can be written as

$$\hat{A}_{n}(t) = e^{iH_{S}t}A_{n}e^{-iH_{S}t}$$

$$= \sum_{a,b} e^{iH_{S}t} |\varepsilon_{a}\rangle \langle \varepsilon_{a}| A_{n} |\varepsilon_{b}\rangle \langle \varepsilon_{b}| e^{-iH_{S}t}$$

$$= \sum_{a,b} e^{-i(\varepsilon_{b}-\varepsilon_{a})t} \langle \varepsilon_{a}|A_{n}|\varepsilon_{b}\rangle |\varepsilon_{a}\rangle \langle \varepsilon_{b}|, \qquad (2.26)$$

defining $\omega := \varepsilon_b - \varepsilon_a$,

$$= \sum_{\omega} e^{-i\omega t} A_n(\omega), \quad \text{where } A_n(\omega) = \sum_{\varepsilon_b - \varepsilon_a = \omega} \langle \varepsilon_a | A_n | \varepsilon_b \rangle | \varepsilon_a \rangle \langle \varepsilon_b | = A_n^{\dagger}(-\omega).$$
(2.27)

With this one obtains

$$[H_{\rm S}, A_n(\omega)] = H_{\rm S} \left(\sum_{\varepsilon_b - \varepsilon_a = \omega} \langle \varepsilon_a | A_n | \varepsilon_b \rangle | \varepsilon_a \rangle \langle \varepsilon_b | \right) - \left(\sum_{\varepsilon_b - \varepsilon_a = \omega} \langle \varepsilon_a | A_n | \varepsilon_b \rangle | \varepsilon_a \rangle \langle \varepsilon_b | \right) H_{\rm S}$$
$$= \sum_{\varepsilon_b - \varepsilon_a = \omega} \langle \varepsilon_a | A_n | \varepsilon_b \rangle | \varepsilon_a \rangle \langle \varepsilon_b | (\varepsilon_a - \varepsilon_b)$$
$$= -\omega A_n(\omega). \tag{2.28}$$

Similarly one finds

$$\left[H_{\rm S}, A_n^{\dagger}(\omega)\right] = \omega A_n^{\dagger}(\omega), \qquad (2.29)$$

$$\left[H_{\rm S}, A_n^{\dagger}(\omega)A_m(\omega)\right] = 0.$$
(2.30)

Getting back to equation (2.25), before plugging in above eigenoperator decompositions, the hermeticity of $\hat{A}_n(t)$ is used to rewrite it to

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -g^2 \sum_{n} \sum_{m} \int_{0}^{\infty} \mathrm{d}\tau \left[\hat{A}_{n}^{\dagger}(t), \hat{A}_{m}(t-\tau)\hat{\rho}_{\mathrm{S}}(t)\right] \bar{B}_{nm}(\tau,0) + \mathrm{h.c.}.$$
(2.31)

Using the above eigenoperator relations and reordering the equation yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -g^2 \sum_{n,m} \sum_{\omega,\omega'} \Gamma_{nm}(\omega') e^{i(\omega-\omega')t} \left[A_n^{\dagger}(\omega), A_m(\omega')\hat{\rho}_{\mathrm{S}}(t) \right] + \mathrm{h.c.}, \qquad (2.32)$$

where $\Gamma_{nm}(\omega') := \int_{0}^{\infty} d\tau \, \bar{B}_{nm}(\tau, 0) e^{i\omega'\tau}$ is a half-range Fourier transformation.

2.3 Secular Approximation

In equation (2.32), there is an oscillating term in front of each commutator. For $t \gg 1/|\omega - \omega'|$, $\omega \neq \omega'$, they are rapidly oscillating. Thus, it is reasonable to use the secular approximation

$$e^{\pm i(\omega-\omega')t} \approx \delta_{\omega,\omega'}.$$
(2.33)

To be consistent with the Markov approximation, it is necessary to impose the constraint [28]

$$\min_{\omega \neq \omega'} |\omega - \omega'| > 1/\tau_{\rm B} \gg g.$$
(2.34)

Overall, there are three time scales which have to fulfill

$$\tau_{\rm R} \gg \tau_{\rm B} > \tau_{\rm S} := \max_{\omega \neq \omega'} \frac{1}{|\omega - \omega'|}.$$
(2.35)

Here, $\tau_{\rm R}$ can be identified with the thermalization time, $\tau_{\rm B}$ is the characteristic time scale for which the bath correlation decays to zero, and $\tau_{\rm S}$ is the time scale of the evolution of the system.

Applying the secular approximation, equation (2.32) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -g^2 \sum_{n,m} \sum_{\omega} \Gamma_{nm}(\omega) \left[A_n^{\dagger}(\omega), A_m(\omega)\hat{\rho}_{\mathrm{S}}(t) \right] + \mathrm{h.c.}.$$
(2.36)

From here on, the only thing left to do is to bring equation (2.36) into Lindblad form.

Considering first $\Gamma_{nm}(\omega)$, one can define the corresponding full Fourier transformation

$$\gamma_{nm}(\omega) := \int_{-\infty}^{\infty} d\tau \, \bar{B}_{nm}(\tau, 0) e^{i\omega\tau}$$

$$= \int_{-\infty}^{0} d\tau \, \bar{B}_{nm}(\tau, 0) e^{i\omega\tau} + \int_{0}^{\infty} d\tau \, \bar{B}_{nm}(\tau, 0) e^{i\omega\tau}$$

$$= \int_{-\infty}^{0} d\tau \, \bar{B}_{nm}(\tau, 0) e^{i\omega\tau} + \Gamma_{nm}(\omega). \qquad (2.37)$$

Claim: The first term on the right-hand side of equation (2.37) obeys $\int_{-\infty}^{0} d\tau \, \bar{B}_{nm}(\tau, 0) e^{i\omega\tau} = \Gamma_{mn}^{*}(\omega).$

Proof:

$$\int_{-\infty}^{0} \mathrm{d}\tau \bar{B}_{nm}(\tau,0) e^{i\omega\tau} = -\int_{0}^{-\infty} \mathrm{d}\tau \,\bar{B}_{nm}(\tau,0) e^{i\omega\tau}, \qquad \text{subst. }\nu := -\tau,$$
$$= \int_{0}^{\infty} \mathrm{d}\nu \,\bar{B}_{nm}(-\nu,0) e^{-i\omega\nu} = \int_{0}^{\infty} \mathrm{d}\nu \,\bar{B}_{mn}^{*}(\nu,0) e^{-i\omega\nu}$$
$$= \left(\int_{0}^{\infty} \mathrm{d}\nu \,\bar{B}_{mn}(\nu,0) e^{i\omega\nu}\right)^{*} = \Gamma_{mn}^{*}(\omega).$$

Thus, one obtains

$$\gamma_{nm}(\omega) = \Gamma_{mn}^*(\omega) + \Gamma_{nm}(\omega). \tag{2.38}$$

Claim: The Fourier transform of $\bar{B}_{nm}(\tau, 0)$ obeys $\gamma_{nm}^*(\omega) = \gamma_{mn}(\omega)$.

Proof:

$$\gamma_{mn}^{*}(\omega) = \int_{-\infty}^{\infty} d\tau \bar{B}_{nm}^{*}(\tau, 0) e^{-i\omega\tau} = \int_{-\infty}^{\infty} d\tau \bar{B}_{mn}(-\tau, 0) e^{-i\omega\tau}, \quad \text{subst. } \nu := -\tau,$$
$$= -\int_{-\infty}^{-\infty} d\nu \bar{B}_{mn}(\nu, 0) e^{i\omega\nu} = \int_{-\infty}^{\infty} d\nu \bar{B}_{mn}(\nu, 0) e^{i\omega\nu} = \gamma_{mn}(\omega).$$

By using the inverse Fourier transformation on $\gamma_{nm}(\omega)$, one can find

$$\bar{B}_{nm}(\tau,0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \,\gamma_{nm}(\omega) e^{-i\omega\tau}.$$
(2.39)

Plugging this back in the half-range Fourier transformation $\Gamma_{nm}(\omega)$ leads to

$$\Gamma_{nm}(\omega) = \int_{0}^{\infty} d\tau \, \bar{B}_{nm}(\tau, 0) e^{i\omega\tau} = \int_{0}^{\infty} d\tau \, e^{i\omega\tau} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \, e^{-i\omega'\tau} \gamma_{nm}(\omega')$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \, \gamma_{nm}(\omega') \int_{0}^{\infty} d\tau \, e^{i(\omega-\omega')\tau}.$$
(2.40)

Using the Sokhotski-Plemelj formula [32]

$$\int_{0}^{\infty} \mathrm{d}x \, e^{\pm ikx} = \lim_{\varepsilon \to 0^{+}} \frac{\pm i}{k \pm i\varepsilon} = \pm i\mathcal{P}\left(\frac{1}{k}\right) + \pi\delta(k) \tag{2.41}$$

with $\mathcal{P}(1/k)$ being the Cauchy principal value one finds

$$\Gamma_{nm}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \gamma_{nm}(\omega') \left[\pi \delta(\omega - \omega') + i\mathcal{P}\left(\frac{1}{\omega - \omega'}\right) \right]$$
$$= \frac{1}{2} \int_{-\infty}^{\infty} d\omega' \gamma_{nm}(\omega') \delta(\omega - \omega') + i \cdot \underbrace{\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \gamma_{nm}(\omega') \mathcal{P}\left(\frac{1}{\omega - \omega'}\right)}_{=: S_{nm}(\omega)}$$
$$= \frac{1}{2} \gamma_{nm}(\omega) + i S_{nm}(\omega). \tag{2.42}$$

Note that $\gamma_{nm}(\omega) = \gamma_{mn}^*(\omega)$ leads to $S_{nm}(\omega) = S_{mn}^*(\omega)$. Combining equations (2.38) and (2.42) yields

$$S_{nm}(\omega) = \frac{1}{2i} \left(\Gamma_{nm}(\omega) - \Gamma_{nm}^*(\omega) \right).$$
(2.43)

Returning to equation (2.36) and rearranging the indices in the hermitian conjugate part, the master equation may be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -g^{2}\sum_{n,m}\sum_{\omega} \left[\Gamma_{nm}(\omega)A_{n}^{\dagger}(\omega)A_{m}(\omega)\hat{\rho}_{\mathrm{S}}(t) - \Gamma_{nm}(\omega)A_{m}(\omega)\hat{\rho}_{\mathrm{S}}(t)A_{n}^{\dagger}(\omega) + \Gamma_{mn}^{*}(\omega)\hat{\rho}_{\mathrm{S}}(t)A_{n}^{\dagger}(\omega)A_{m}(\omega) - \Gamma_{mn}^{*}(\omega)A_{m}(\omega)\hat{\rho}_{\mathrm{S}}(t)A_{n}^{\dagger}(\omega)\right].$$
(2.44)

Using equations (2.42) and (2.43), as well as $\gamma_{mn}^*(\omega) = \gamma_{nm}(\omega)$ and $S_{mn}^*(\omega) = S_{nm}(\omega)$, the master equation can be written in Lindblad form

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -i\left[H_{\mathrm{LS}},\hat{\rho}_{\mathrm{S}}(t)\right] + g^{2}\sum_{n,m}\sum_{\omega}\gamma_{nm}(\omega)\left(A_{m}(\omega)\hat{\rho}_{\mathrm{S}}(t)A_{n}^{\dagger}(\omega) - \frac{1}{2}\left\{A_{n}^{\dagger}(\omega)A_{m}(\omega),\hat{\rho}_{\mathrm{S}}(t)\right\}\right)$$
(2.45)

with $H_{\rm LS} = g^2 \sum_{n,m} \sum_{\omega} S_{nm}(\omega) A_n^{\dagger}(\omega) A_m(\omega)$, the Lamb shift Hamiltonian. Note that equation (2.30) implies $[H_{\rm LS}, H_{\rm S}] = 0$.

Transforming equation (2.45) to the Schrödinger picture, one gets

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}}(t) = -i\left[H_{\mathrm{S}} + H_{\mathrm{LS}}, \rho_{\mathrm{S}}(t)\right] + g^{2}\sum_{n,m}\sum_{\omega}\gamma_{nm}(\omega)\left(A_{m}(\omega)\rho_{\mathrm{S}}(t)A_{n}^{\dagger}(\omega) - \frac{1}{2}\left\{A_{n}^{\dagger}(\omega)A_{m}(\omega), \rho_{\mathrm{S}}(t)\right\}\right).$$
(2.46)

To show that the positivity of the density matrix is preserved, one needs to show $\gamma(\omega) > 0$. A proof can be found in the lecture notes of Lidar [28]. It uses Bochner's theorem, for which a proof can be found in [33].

2.4 The KMS Condition

The Kubo-Martin-Schwinger (KMS) condition is a kind of boundary-value condition which is important to formalize the notion that systems tend to relax into lower energy states.

The relation

$$\langle \hat{B}_n(t)\hat{B}_m(t')\rangle = \langle \hat{B}_n(t-t')\hat{B}_m(0)\rangle, \qquad (2.47)$$

implies

$$\langle \hat{B}_n(t+\tau)\hat{B}_m(t)\rangle = \langle \hat{B}_n(\tau)\hat{B}_m\rangle.$$
(2.48)

This means that the bath-correlation function is time-translation invariant. According to Lidar [28], if the bath state in this function is not only stationary, but also in thermal equilibrium at inverse temperature β , then it holds that

$$\langle \hat{B}_n(\tau)\hat{B}_m(0)\rangle = \langle \hat{B}_m(0)\hat{B}_n(\tau+i\beta)\rangle = \langle \hat{B}_m(-\tau-i\beta)\hat{B}_n(0)\rangle, \qquad (2.49)$$

which is known as the KMS condition. If additionally the correlation function is analytic, then the KMS condition can be expressed in the frequency domain as

$$\gamma_{nm}(-\omega) = \gamma_{mn}(\omega)e^{-\beta\omega}.$$
(2.50)

The above relation shows that excitations in the system are exponentially supressed relative to the corresponding relaxations at the same frequencies. Moreover, Kossakowski et al. [34] have shown that a system weakly coupled to a reservoir, which obeys the KMS condition, shows detailed balance which means, that all appearing coherences in $\rho_{\rm S}(t)$ vanish over time, such that it is sufficient to consider the populations only, i.e. the diagonal entries of $\rho_{\rm S}(t)$.

3 Non-Interacting Collective-Spin Model in a Quantum Otto Cycle

In this section, some results of the paper of Kloc, Cejnar, and Schaller [26] are shown, that are important for this work. Any additional sources are indicated in the text.

3.1 Quantum Otto Cycle

The quantum Otto cycle, as depicted in Figure 3.1, consists of four strokes. The medium used for the cycle is called working fluid. It usually is made up of an ensemble of particles, whose state can be described in the density matrix formalism. Suppose the state of the ensemble is fully thermalized at a cold initial temperature T_c (position 1 in Figure 3.1). The first stroke $(1 \rightarrow 2)$ is a unitary transformation, in which only a dimensionless control parameter λ_i gets changed to λ_f . According to Wilde [35], the (von Neumann) entropy remains invariant under this transformation. The first stroke can be understood as a rescaling in the energy levels without inducing any changes in the distribution of the occupation probabilities. At position 2 in the cycle, the working fluid gets coupled to a hot reservoir (stroke $2 \rightarrow 3$). The control parameter λ_f remains unchanged, but due to thermalization the particles in the ensemble undergo transitions of their respective energy levels, leading to a change in entropy. The third stroke $(3 \rightarrow 4)$ is again a unitary transformation where the control parameter λ_f assumes the initial value λ_i . In the last stroke $(4 \rightarrow 1)$ the system gets coupled to a cold reservoir.



Figure 3.1: Schematic representation of the quantum Otto cycle. S is the (von Neumann) entropy and λ is the dimensionless control parameter. Q_h is the heat that gets transferred from the hot thermal reservoir with temperature T_h to the ensemble, and Q_c corresponds to the heat transfer from the ensemble to the cold heat reservoir with temperature T_c respectively. This figure is a combination of two figures, from [26] and [36].

The heat transfer from the heat baths to the working fluid (Q_h) and vice versa (Q_c) during the thermalizations can be expressed as

$$Q_h = \langle E_3 \rangle - \langle E_2 \rangle = \operatorname{Tr} \left(H_f \rho_3 \right) - \operatorname{Tr} \left(H_f \rho_2 \right) = \operatorname{Tr} \left(H_f \left(\rho_3 - \rho_2 \right) \right) > 0, \tag{3.1}$$

$$Q_c = \langle E_1 \rangle - \langle E_4 \rangle = \operatorname{Tr} (H_i \rho_1) - \operatorname{Tr} (H_i \rho_4) = \operatorname{Tr} (H_i (\rho_1 - \rho_4)) < 0.$$
(3.2)

Here the indices $\{1, 2, 3, 4\}$ denote the positions in the quantum Otto cycle as shown in Figure 3.1. Furthermore, $H_f = H(\lambda_f)$, and $H_i = H(\lambda_i)$, where H describes the Hamiltonian of the ensemble. The total work per cycle can be determined using the first law of thermodynamics,

$$W = -(Q_h + Q_c).$$
 (3.3)

For simplicity the work is calculated with W' := -W. Thus, the efficiency of the quantum Otto cycle is given by

$$\eta = \frac{W'}{Q_h} = \frac{Q_h + Q_c}{Q_h} = 1 + \frac{Q_c}{Q_h} = 1 - \frac{|Q_c|}{Q_h}.$$
(3.4)

The efficiency is bounded by the Carnot efficiency, i.e. $\eta \leq \eta_C = 1 - T_c/T_h$.

3.2 Non-Interacting Collective-Spin Model as Working Fluid

Consider an ensemble of N identical non-interacting two-level systems (e.g. qubits), described by the Hamiltonian

$$H(t) = \lambda(t)\omega_0 J_z, \tag{3.5}$$

where λ is a dimensionless control parameter, ω_0 is an energy scaling factor, and J_z a collective-spin operator,

$$J_z = \sum_{i=1}^{N} \frac{\sigma_i^z}{2},$$
 (3.6)

where σ^z is a Pauli matrix. Due to this formalism, the number of two-level systems can be expressed as N = 2j (see Appendix A). In the present work, this working fluid is also called linear model, because the system Hamiltonian (3.5) is linear with respect to the collective-spin operator J_z .

For the non-unitary thermalization strokes of the quantum Otto cycle the following Lindblad master equation is used:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = -i\lambda\omega_0 \left[J_z,\rho\right] + \gamma(1+n_b)\mathcal{D}\left[J_-\right]\rho + \gamma n_b\mathcal{D}\left[J_+\right]\rho.$$
(3.7)

Here, γ is a constant dissipation rate, $n_b = (e^{\beta\lambda} - 1)^{-1}$ with $\beta = 1/T$ is the temperature dependent Bose-Einstein distribution factor, and $\mathcal{D}[O]\rho = O\rho O^{\dagger} - \frac{1}{2} \{O^{\dagger}O, \rho\}$ denotes a Lindblad dissipator for an arbitrary operator O. The jump operators appearing in the Lindblad dissipators are collective operators defined with $J_{\pm} := J_x \pm i J_y$.

According to Breuer and Petruccione [27], Gibbs states of the form

$$\rho_{\rm th} = \frac{e^{-\beta H}}{\operatorname{Tr}\left(e^{-\beta H}\right)} \tag{3.8}$$

are stationary solutions to such a Lindblad master equation. Thus, any initial state ρ_i relaxes to $\rho_{\rm th}$ for $t \to \infty$. This means that full thermalization is only possible for an infinite coupling time, which is not achievable. However, one can introduce a tolerance, for which one accepts a finitely thermalized state as fully thermalized. In order to do so, the quantum relative entropy can be used, since it measures the closeness of two states (see Appendix B). In the remainder of this work, whenever a fully thermalized state is mentioned, it refers to a state sufficiently close, i.e. within tolerance to $\rho_{\rm th}$.

Unitary transformations change the scaling in the energy levels, but leave the von Neumann entropy unchanged. Kloc, Cejnar, and Schaller have shown that the unitary strokes can be done by mapping the temperatures of the states as

$$1 \longrightarrow 2: \quad T_c \mapsto T'_c = \frac{\lambda_f}{\lambda_i} T_c,$$

$$3 \longrightarrow 4: \quad T_h \mapsto T'_h = \frac{\lambda_i}{\lambda_f} T_h.$$
(3.9)

Before the quantum Otto cycle was numerically implemented, the Lindblad master equation (3.7) was tested to ensure that the time evolution of an initial Gibbs state approaches a fully thermalized Gibbs state at another temperature. Hence, two states were initialized, one fully thermalized to the cold reservoir, and one fully thermalized to the hot reservoir. Then the master equation was numerically solved and the quantum relative entropy of the respective states was plotted. As one can see in Figure 3.2, the initial state ρ_i approaches the fully thermalized state $\rho_{\rm th}$ for a long enough coupling time.



Figure 3.2: (a): Quantum relative entropy over time of an initial Gibbs state ρ_i at temperature $T_c = \omega_0$ with respect to a fully thermalized state $\rho_{\rm th}$. The hot reservoir has a temperature of $T_h = 8\omega_0$ and the dimensionless control parameter is set to $\lambda_f = 3$. (b): Quantum relative entropy over time of an initial Gibbs state ρ_i at temperature $T_h = 8\omega_0$ with respect to a fully thermalied state $\rho_{\rm th}$. The cold reservoir has a temperature of $T_c = \omega_0$, and the dimensionless control parameter is $\lambda_i = 1$. In both settings are j = 20, and $\gamma = 0.1\omega_0$

Employing the full quantum Otto cycle, one can see that for a finite coupling time, the engine goes to a 'converged cycle'. Note that this cycle is not stable, as it is sensitive to perturbations of any parameter. Thus, assuming the heat engine operates in a converged cycle, if a temperature of any of the heat baths or the coupling time gets varied, then the quantum Otto cycle will operate towards a new converged cycle. Although the control parameter is periodically changed in time, if its periodicity was changed, then the heat engine would work towards a new converged cycle as well. Choosing the same setup as in Figure 3.2 for both thermalization strokes, as well as the control parameters, and initializing the engine at a Gibbs state at the same temperature as the cold reservoir, the quantum Otto cycle has been plotted once for full thermalization during the thermal strokes (see Figure 3.3a) and once for a finite thermalization (see Figure 3.3b). In the latter one can clearly see that the heat engine goes to a converged cycle for a coupling time shorter than required for full thermalization.

It is important to ensure that the heat engine is already in the converged cycle before one determines the power for coupling times shorter than necessary for full thermalization. This is due to different powers in the cycles previous to the converged one. As long as the setting parameters are unperturbed, the engine will eventually reach the converged cycle and continue to operate in it. Thus for practical reasons, it is beneficial to do further calculations always under the condition that the heat engine already operates in a converged cycle.

To determine the efficiency of the quantum Otto cycle, equation (3.4) is used. The unitary strokes do not change the entropy of the states, as the distribution of occupation probabilities remains. Thus, the density matrices at the positions 1 and 2, as shown in Figure 3.1, are identical, $\rho_1 = \rho_2$. The same applies for the density matrices at positions 3 and 4, yielding $\rho_3 = \rho_4$. Therefore, the efficiency

becomes

$$\eta = 1 + \frac{Q_c}{Q_h} = 1 + \frac{\text{Tr}\left(H_i(\rho_3 - \rho_1)\right)}{\text{Tr}\left(H_f(\rho_1 - \rho_3)\right)} = 1 + \frac{\text{Tr}\left(\lambda_i\omega_0 J_z(\rho_3 - \rho_1)\right)}{\text{Tr}\left(\lambda_f\omega_0 J_z(\rho_1 - \rho_3)\right)} = 1 - \frac{\lambda_i}{\lambda_f} \frac{\text{Tr}\left(\omega_0 J_z(\rho_1 - \rho_3)\right)}{\text{Tr}\left(\omega_0 J_z(\rho_1 - \rho_3)\right)} = 1 - \frac{\lambda_i}{\lambda_f}.$$
(3.10)



Figure 3.3: (a): Quantum Otto cycle with full thermalization during the thermal strokes. The circled numbers represent the positions in the engine as shown in Figure 3.1. (b): The dashed line represents the cycle with full thermalization as shown in (a). The black solid lines show the cycles that were necessary to reach the converged cycle, which is highlighted in red. The coupling time was chosen to be $t\omega_0 = 0.1$.

The duration of a thermalization process until full thermalization is called thermalization time and is dependent on the number of two-level systems, and therefore on j. To demonstrate the dependence, a numerical calculation was done and plotted in Figure 3.4.



Figure 3.4: Dependence of the thermalization time on j. For the thermalization process, the system was initialized at a temperature $T_h = 4\omega_0$ and was cooled down to $T_c = \omega_0$. The control parameters were chosen to be $\lambda_i = 1$, $\lambda_f = 3$, and $\gamma = 0.1\omega_0$. A fit was added to the data, showing that the thermalization time is proportional to 1/j.

The thermalization can be understood as a change of the occupation probability among the 2j + 1energy levels. Due to the linearity of $H_{\rm S}$ in J_z , all levels are equidistantly spaced. In the non-unitary part of equation (3.7), the collective operators J_{\pm} act as one would expect, i.e. J_+ is responsible for going up a level and thus implying some excitation in the ensemble, whereas J_- is responsible for going down a level, hence bringing the system closer to its collective ground state. As the number of energy levels is proportional to j, more energy is needed to occupy higher levels with increasing j. This means that for larger j it is more probable, that even before a thermalization has taken place, the two-level systems in the ensemble are closer to the collective ground state than for smaller j. It also means that for larger j even after the thermalization (depending on the temperature of the heat bath) not too many changes in the occupations of the energy levels are expected. Thus, for increasing j the thermalization time is expected to decrease.

According to Figure 3.4, the thermalization time is proportional to 1/j. This reciprocal dependence implies a superradiant effect for small j. For smaller values of j, there are less energy levels. Thus, the actual energy difference between the ground state and the maximally excited collective state is smaller than for larger j. This results in higher occupation probabilities of higher excited states in smaller systems and thus, through the coherent dissipation, in a superradiant energy emission.

To underline this superradiant effect, the power output of the heat engine dependent on j has been determined. For this, a finite coupling time of $t\omega_0 = 1$ for the thermal strokes has been chosen. Since the unitary strokes in this setting can be arbitrarily fast, the total power of a work cycle is computed with $P = W'_c/t_c$, where $t_c = 2t\omega_0$. The dimensionless control parameters were set to $\lambda_i = 1$, and $\lambda_f = 3$, and the dissipation rate was $\gamma = 0.1\omega_0$. The system was initialized at a temperature of the cold reservoir, $T_c = \omega_0$. The power was calculated for two different temperatures of the hot reservoir, those being $T_h = 40\omega_0$, and $T_h = 80\omega_0$. The resulting plot is shown in Figure 3.5.



Figure 3.5: Power of the collective-spin heat engine as a function of j. The coupling time is fixed to $t\omega_0 = 1$. A quadratic fit was added for $j \leq 5$, implying the proportionality of j^2 for small systems. The dotted line at $P \approx 12.26\omega_0^2$ for $T_h = 40\omega_0$ is the limit of the maximally possible power at that temperature.

In Figure 3.5, there is a quadratic scaling of the power for small values of j. Due to j = N/2, this proportionality to N^2 can be compared to a superradiant emission intensity (see Appendix A). For larger j the quadratic scaling flattens to a linear dependence and then saturates for large j. Because of the saturation, there is a necessity of a large temperature difference between the two heat reservoirs. Otherwise the curve has a smaller maximally possible power and goes faster into the linear growth

and saturation, so that hardly a quadratic scaling is observable. The superradiant scaling for small values of j can be explained as it was mentioned for the thermalization-time dependence on j. If the temperature difference of the initialized state to the hot reservoir is sufficiently large then there is enough potential heat there to occupy higher energy levels. For higher values of j, the energy difference to the maximally excited collective state gets too large such that the respective occupation probability gets smaller, hence a linear growth in the power output. At some point this difference is large enough that the corresponding power output saturates. The limit in power for $j \rightarrow \infty$ can be seen more clearly by plotting the power of the heat engine as a function of coupling time for different values of j. Setting the temperatures of the heat baths to $T_c = \omega_0$ and $T_h = 8\omega_0$, and letting all other parameters as in Figure 3.5, the power dependent on coupling time is plotted in Figure 3.6.



Figure 3.6: Dependence of the power of a converged cycle on coupling time for different values of j. The dotted line represents the coupling time used for Figure 3.5.

According to Figure 3.6, there is a finite power in the limit $j \rightarrow \infty$. This limit can be calculated analytically [26],

$$\lim_{j \to \infty} \frac{W_c'}{t_c} = \frac{(\lambda_f - \lambda_i)\omega_0}{2t\omega_0} \frac{e^{\lambda_i\omega_0/T_c} - e^{\lambda_f\omega_0/T_h}}{\left(e^{\lambda_f\omega_0/T_h} - 1\right)\left(e^{\lambda_i\omega_0/T_c} - 1\right)}.$$
(3.11)

It is also evident from Figure 3.6 that short coupling times are beneficial for the power. For coupling times larger than required for full thermalization, no additional power can be extracted anymore and any longer coupling to the heat bath would just reduce the power proportional to $1/t\omega_0$.

To see the occuring superradiance more on a mathematical level, equation (3.7) can be expressed in terms of the eigenbasis $J_z |m\rangle = m |m\rangle$ to find $\langle n|\dot{\rho}|m\rangle$. All elements for which $n \neq m$ evolve independently from the diagonal elements and decay to zero. Using the notation $\rho_m := \langle m|\rho|m\rangle$, the thermalization is given with the rate equation

$$\dot{\rho}_{m} = \gamma (1+n_{b})(j+m)(j-m+1)\rho_{m-1} + \gamma n_{b}(j-m)(j+m+1)\rho_{m+1} - \gamma (1+n_{b}) \left[j(j+1) - m(m+1) \right] \rho_{m} - \gamma n_{b} \left[j(j+1) - m(m-1) \right] \rho_{m}.$$
(3.12)

Equation (3.12) reveals proportionalities to j^2 for m = 0, as required for a superradiant scaling. If $m \neq 0$, there are linear proportionalities only. Although the quadratic scaling appears rigorously just for m = 0, the scaling can be regarded as superradiant for $m \approx 0$, as the Clebsch-Gordan coefficients are still large compared to the regime, where $m \approx \pm j$.

4 Interacting Collective-Spin Model

Let the working fluid be the same collective-spin model as before, but the collective-spin operator becomes squared, thus introducing an infinite-range interaction among the two-level systems. Hence, the Hamiltonian of the ensemble is written as

$$H_{\rm S}(t) = \lambda(t)\omega_0 J_z^2. \tag{4.1}$$

In the present work, due to the proportionality to J_z^2 this working fluid is also called quadratic model. Because of the squared collective-spin operator the energy levels are not equidistantly distributed anymore. Instead, they space quadratically. This means that the previous Lindblad master equation (3.7) cannot be applied for this working fluid. Hence, there is a need to derive another master equation to describe the thermal strokes in the quantum Otto cycle.

To be able to derive such an equation, there is a need to have a model for the thermal reservoirs, as well as the interaction between them and the working fluid. Each heat bath is chosen to be made of bosonic harmonic oscillators. This type of bath is a typical choice and commonly used for systems, that are weakly coupled to their environment [37]. Thus, the respective Hamiltonian is given by

$$H_{\rm B} = \sum_{k} \omega_k b_k^{\dagger} b_k. \tag{4.2}$$

The additional term of +1/2 that usually appears in Hamiltonians of harmonic oscillators only causes a small shift in the eigenenergy levels of the heat bath and can be omitted.

The interaction between a heat bath and the working fluid is modelled with

$$H_{\rm I} = J_x \otimes \sum_k \left(h_k b_k + h_k^* b_k^\dagger \right), \tag{4.3}$$

where the h_k represent the mode strengths of the bosonic bath oscillators. This interaction type is in analogy to Dicke's model, where a dipole approximation was made to describe the interaction between an electromagnetic radiating field and an emsemble consisting of two-level systems. The collectivespin operator J_x can be written in terms of J_+ and J_- , leading to a description of transitions in the occupation-probability distribution in the ensemble. A derivation for an interaction Hamiltonian for a system like Dicke's model can be found in [38].

4.1 Derivation of the Master Equation

To find an equation to describe the thermalization process in the case of an interacting collective-spin model coupled to a heat bath, a similar procedure is applied as in Section 2. Most calculations are completely analogous. Thus, in the derivation, only important intermediate results are presented here. More technical details can be found in Appendix C.

Like equation (2.3), the interaction picture is used to write the von Neumann equation as

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}(t) = -i\left[\hat{H}(t), \hat{\rho}(t)\right],\tag{4.4}$$

with

$$\hat{\rho}(t) = e^{i(H_{\rm S} + H_{\rm B})t} \rho e^{-i(H_{\rm S} + H_{\rm B})t},\tag{4.5}$$

$$\hat{H}(t) = \hat{J}_x \otimes \hat{B}. \tag{4.6}$$

Here, the operators in equation (4.6) are

$$\hat{J}_x = e^{iH_{\rm S}t} J_x e^{-iH_{\rm S}t},\tag{4.7}$$

$$\hat{B} := e^{iH_{\rm B}t} \sum_{k} \left(h_k b_k + h_k^* b_k^\dagger \right) e^{-iH_{\rm B}t} = \sum_{k} h_k e^{-i\omega_k t} b_k + h_k^* e^{i\omega_k t} b_k^\dagger.$$
(4.8)

Equation (4.4) can be recast in its integral form and rearranged to

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}(t) = -i\left[\hat{H}(t),\hat{\rho}(0)\right] - \int_{0}^{t} \mathrm{d}t'\left[\hat{H}(t),\left[\hat{H}(t'),\hat{\rho}(t')\right]\right].$$
(4.9)

4.1.1 Born Approximation

Assume the external reservoir is a heat bath sufficiently large, such that effects of the system on the heat bath are negligible. This allows to separate the degrees of freedom in the density matrix and hence the usage of the Born approximation $\hat{\rho}(t) \approx \hat{\rho}_{\rm S}(t) \otimes \hat{\rho}_{\rm B}$ with $\hat{\rho}_{\rm B}$ being a stationary Gibbs state of the bath.

Using this approximation, plugging in the expression (4.6) for $\hat{H}(t)$, and tracing out the bath is done analogously as in Section 2.1, yielding

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -\int_{0}^{t} \mathrm{d}\tau \left(\left[\hat{J}_{x}(t), \hat{J}_{x}(t-\tau)\hat{\rho}_{\mathrm{S}}(t-\tau) \right] \langle \hat{B}(\tau)\hat{B}(0) \rangle + \mathrm{h.c.} \right), \tag{4.10}$$

where the new variable $\tau := t - t'$ and the bath-correlation function $\langle \hat{B}(\tau)\hat{B}(0)\rangle = \text{Tr}\left(\hat{B}(\tau)\hat{B}(0)\hat{\rho}_{\text{B}}\right)$ were introduced.

4.1.2 On the Bath-Correlation Function

The bath-correlation function contains a discrete sum and is given by

$$\langle \hat{B}(\tau)\hat{B}(0)\rangle = \sum_{k} |h_{k}|^{2} \bigg[e^{-i\omega_{k}\tau} \left(1 + n_{b}(\omega_{k})\right) + e^{i\omega_{k}\tau} n_{b}(\omega_{k}) \bigg], \qquad (4.11)$$

where $n_b(\omega_k)$ is the Bose-Einstein distribution factor

$$n_b(\omega_k) = \left(e^{\omega_k\beta} - 1\right)^{-1} \tag{4.12}$$

with the inverse temperature β . Following Schaller [30] and going to the continuous case, and defining a spectral density

$$J(\omega) := 2\pi \sum_{k} |h_k|^2 \delta(\omega - \omega_k) \tag{4.13}$$

gives

$$\langle \hat{B}(\tau)\hat{B}(0)\rangle = \frac{1}{2\pi} \int_{0}^{\infty} d\omega J(\omega) \left(e^{-i\omega\tau} \left(1 + n_{b}(\omega)\right) + e^{i\omega\tau} n_{b}(\omega) \right).$$
(4.14)

The spectral density is defined for positive frequencies, but can be analytically continued to negative frequencies by defining $J(-\omega) := -J(\omega)$. Using this and

$$n_{b}(-\omega) = \frac{1}{e^{-\omega\beta} - 1} = \frac{-e^{\omega\beta}}{e^{\omega\beta} - 1} = \frac{-e^{\omega\beta} + 1 - 1}{e^{\omega\beta} - 1} = \frac{-(e^{\omega\beta} - 1)}{e^{\omega\beta} - 1} - \frac{1}{e^{\omega\beta} - 1} = -\left(1 + \frac{1}{e^{\omega\beta} - 1}\right) = -\left(1 + n_{b}(\omega)\right),$$
(4.15)

the bath-correlation function can be rewritten by first splitting the integral,

$$\langle \hat{B}(\tau)\hat{B}(0)\rangle = \frac{1}{2\pi} \int_{0}^{\infty} d\omega J(\omega)e^{-i\omega\tau} \left(1 + n_{b}(\omega)\right) + \frac{1}{2\pi} \int_{0}^{\infty} d\omega J(\omega)e^{i\omega\tau}n_{b}(\omega),$$

and substituting $\omega \longrightarrow -\omega$ in the second integral,

$$= \frac{1}{2\pi} \int_{0}^{\infty} d\omega J(\omega) e^{-i\omega\tau} \left(1 + n_{b}(\omega)\right) + \frac{1}{2\pi} \int_{0}^{-\infty} (-d\omega) J(-\omega) e^{-i\omega\tau} n_{b}(-\omega)$$

$$= \frac{1}{2\pi} \int_{0}^{\infty} d\omega J(\omega) e^{-i\omega\tau} \left(1 + n_{b}(\omega)\right) + \frac{1}{2\pi} \int_{-\infty}^{0} d\omega J(\omega) e^{-i\omega\tau} \left(1 + n_{b}(\omega)\right)$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega J(\omega) e^{-i\omega\tau} \left(1 + n_{b}(\omega)\right).$$
(4.16)

Defining $\gamma(\omega) := J(\omega)(1 + n_b(\omega))$, the bath-correlation function $\langle \hat{B}(\tau)\hat{B}(0)\rangle$ is its inverse Fourier transform, implying that $\gamma(\omega)$ can also be written as the Fourier transform

$$\gamma(\omega) = \int_{-\infty}^{\infty} \mathrm{d}\tau \, \langle \hat{B}(\tau) \hat{B}(0) \rangle e^{i\omega\tau}.$$
(4.17)

Because of the divergence of $n_b(\omega)$ for $\omega \to 0$, it is reasonable to choose a parametrization of $J(\omega)$ that ensures a finite value of $\gamma(\omega)$ in this limit. Using a phenomenological approach [39], a so-called ohmic spectral density is chosen, i.e.

$$J(\omega) = J_0 \omega e^{-\omega/\omega_c},\tag{4.18}$$

where J_0 is the strength of the collective coupling to the bath and ω_c is a cut-off frequency, ensuring that the high frequency couplings do not diverge. This choice of spectral density grows approximately linearly up to ω_c and then decays exponentially. The idea behind this choice is that mainly low frequencies of the thermal bath contribute to physical processes in the interaction with the system. It is important that the spectral density decays for higher frequencies, since this causes the bath-correlation function to decay in time. This is especially important in weakly coupled systems.

To see that with this choice of the ohmic spectral density the bath-correlation function decays over time, the inverse Fourier transform (4.16) needs to be evaluated. This can be done analytically. Plugging in equation (4.18) and using equation (4.15) allows to write the integral as

$$\langle \hat{B}(\tau)\hat{B}(0)\rangle = -\frac{J_0}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega \,\omega e^{-\omega(1/\omega_c + i\tau)} \,\frac{1}{e^{-\beta\omega} - 1}.\tag{4.19}$$

Substituting $\omega := -x$, defining $\mu := 1/\omega_c + i\tau$, and $\nu := \beta$ leads to the representation

$$\langle \hat{B}(\tau)\hat{B}(0)\rangle = \frac{J_0}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}x \, \frac{x e^{\mu x}}{e^{\nu x} - 1}.$$
 (4.20)

This form of integral and its solution can be found in [40]:

$$\langle \hat{B}(\tau)\hat{B}(0)\rangle = \frac{J_0}{2\pi} \left(\frac{\pi}{\nu} \operatorname{cosec}\left(\frac{\mu\pi}{\nu}\right)\right)^2, \quad \operatorname{Re}(\nu) > \operatorname{Re}(\mu) > 0.$$
(4.21)

Substituting back the definitions for μ and ν , and making use of $\operatorname{cosech}(x + iy) = i\operatorname{cosech}(ix - y)$ and $\operatorname{cosech}(-x) = -\operatorname{cosech}(x)$ for all $x, y \in \mathbb{R}$, this expression can be brought into the following form

$$\langle \hat{B}(\tau)\hat{B}(0)\rangle = -\frac{J_0\pi}{2\beta^2}\operatorname{cosech}^2\left(\frac{\tau\pi}{\beta} - i\frac{\pi}{\omega_c\beta}\right), \quad \omega_c > \beta^{-1}.$$
(4.22)

Both the spectral density and the bath-correlation function have been plotted in Figure 4.1. For both plots a cut-off frequency of $\omega_c = 100\omega_0$, and $J_0 = 1$ have been used. Additionally the temperature in the bath-correlation function was set to $T = 25\omega_0$. The ohmic spectral density $J(\omega)$ (Figure 4.1a) has, compared to the bath-correlation function (Figure 4.1b), a much wider range on the axis of abscissa. This is due to their relation by a Fourier transformation. Therefore, this behaviour becomes stronger, the larger ω_c is chosen. To ensure that the later applied Markov approximation is not violated $J_0 = 1$, and $\omega_c = 500\omega_0$ are chosen for all calculations.



Figure 4.1: (a): Ohmic spectral density as described in equation (4.18). It grows approximately linearly until it peaks at ω_c . For $\omega > \omega_c$ it decays exponentially. (b): Bath-correlation function (4.22) at $T = 25\omega_0$. Because of the complex argument in the hyperbolic cosecant, the real and imaginary part of the function are depicted separately. In both plots $J_0 = 1$ and $\omega_c = 100\omega_0$.

The choice of the parametrization of $J(\omega)$ has to ensure a finite value of $\gamma(\omega)$ for $\omega \longrightarrow 0$. This limit does exist and is given by

$$\lim_{\omega \to 0} \gamma(\omega) = \frac{J_0}{\beta} = J_0 T.$$
(4.23)

4.1.3 Markov Approximation

Returning to equation (4.10), the Markov approximation can be applied just like in the derivation of the Lindblad master equation in Section 2.2. Assuming weak coupling and rapidly decaying bath correlations compared to the relaxation time of the system, the bath obtains a 'short-memory'. Similar to equation (2.25), the upper limit of the integral can be set to infinity and $\hat{\rho}_{\rm S}(t-\tau)$ can be replaced with $\hat{\rho}_{\rm S}(t)$, such that equation (4.10) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -\int_{0}^{\infty} \mathrm{d}\tau \left(\left[\hat{J}_{x}(t), \hat{J}_{x}(t-\tau)\hat{\rho}_{\mathrm{S}}(t) \right] \langle \hat{B}(\tau)\hat{B}(0) \rangle + \mathrm{h.c.} \right).$$
(4.24)

Since this is a Redfield master equation, it still does not guarantee the positivity of $\hat{\rho}_{\rm S}(t)$. Thus, a further approximation is applied, namely the secular approximation. But before its implementation, the same steps are performed in complete analogy to Section 2.2, i.e. the eigenoperator decomposition of $\hat{J}_x(t)$ is used. Thus, equation (4.24) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -\sum_{\omega}\sum_{\omega'} \left[\Gamma(\omega')e^{i(\omega-\omega')t} \left[J_x^{\dagger}(\omega), J_x(\omega')\hat{\rho}_{\mathrm{S}}(t) \right] + \mathrm{h.c.} \right],\tag{4.25}$$

where $\Gamma(\omega') := \int_{0}^{\infty} d\tau \langle \hat{B}(\tau) \hat{B}(0) \rangle e^{i\omega'\tau}$ is a half-range Fourier transformation.

4.1.4 Secular Approximation

Just like in Section 2.3, each commutator in equation (4.25) is linked with a rapidly oscillating term for $t \gg 1/|\omega - \omega'|$, $\omega \neq \omega'$. Since these terms are responsible for a possible violation of the positivity of $\hat{\rho}_{\rm S}(t)$, a secular approximation is applied by setting $e^{\pm i(\omega - \omega')t} \approx \delta_{\omega,\omega'}$. With this equation (4.25) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -\sum_{\omega} \bigg[\Gamma(\omega) \left[J_x^{\dagger}(\omega), J_x(\omega)\hat{\rho}_{\mathrm{S}}(t) \right] + \mathrm{h.c.} \bigg].$$
(4.26)

To bring equation 4.26 in Lindblad form,

$$\gamma(\omega) = \int_{-\infty}^{\infty} d\tau \, \langle \hat{B}(\tau) \hat{B}(0) \rangle e^{i\omega\tau} = \Gamma^*(\omega) + \Gamma(\omega)$$
(4.27)

$$\sigma(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \gamma(\omega') \mathcal{P}\left(\frac{1}{\omega - \omega'}\right) = \frac{1}{2i} \left(\Gamma(\omega) - \Gamma^*(\omega)\right), \qquad (4.28)$$

whose derivations are analogous to those in Section 2.3, are used. The master equation is then given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -i\left[H_{\mathrm{LS}},\hat{\rho}_{\mathrm{S}}(t)\right] + \sum_{\omega}\gamma(\omega)\left(J_{x}(\omega)\hat{\rho}_{\mathrm{S}}(t)J_{x}^{\dagger}(\omega) - \frac{1}{2}\left\{J_{x}^{\dagger}(\omega)J_{x}(\omega),\hat{\rho}_{\mathrm{S}}(t)\right\}\right),\tag{4.29}$$

with the Lamb-shift Hamiltonian $H_{\rm LS} = \sum_{\omega} \sigma(\omega) J_x^{\dagger}(\omega) J_x(\omega).$

Transforming it back to the Schrödinger picture yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}}(t) = -i\left[H_{\mathrm{S}} + H_{\mathrm{LS}}, \rho_{\mathrm{S}}(t)\right] + \sum_{\omega}\gamma(\omega)\left(J_{x}(\omega)\rho_{\mathrm{S}}(t)J_{x}^{\dagger}(\omega) - \frac{1}{2}\left\{J_{x}^{\dagger}(\omega)J_{x}(\omega), \rho_{\mathrm{S}}(t)\right\}\right).$$
(4.30)

Note that the commutation relation $\left[H_{\rm S}, J_x^{\dagger}(\omega)J_x(\omega)\right] = 0$ immediately implies $\left[H_{\rm S}, H_{\rm LS}\right] = 0$.

For a more general representation of the master equation (4.30), a new notation is introduced,

$$J_x(\omega) = \sum_{\varepsilon_b - \varepsilon_a = \omega} \langle \varepsilon_a | J_x | \varepsilon_b \rangle | \varepsilon_a \rangle \langle \varepsilon_b | = \sum_{\varepsilon_b - \varepsilon_a = \omega} J_x^{ab} L_{ab},$$
(4.31)

where $J_x^{ab} := \langle \varepsilon_a | J_x | \varepsilon_b \rangle$ and $L_{ab} := | \varepsilon_a \rangle \langle \varepsilon_b |$. With these definitions, equation (4.30) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}}(t) = -i\left[H_{\mathrm{S}} + H_{\mathrm{LS}}, \rho_{\mathrm{S}}(t)\right] + \sum_{\substack{a,b,\\c,d}} \gamma_{ab,cd} \left(L_{ab}\rho_{\mathrm{S}}(t)L_{cd}^{\dagger} - \frac{1}{2}\left\{L_{cd}^{\dagger}L_{ab}, \rho_{\mathrm{S}}(t)\right\}\right),\tag{4.32}$$

where $\gamma_{ab,cd} = \gamma(\varepsilon_b - \varepsilon_a) \delta_{\varepsilon_b - \varepsilon_a, \varepsilon_d - \varepsilon_c} J_x^{ab} (J_x^{cd})^*$. The Kronecker delta was inserted to ensure the secular approximation. In this notation the Lamb-shift Hamiltonian takes the form

$$H_{\rm LS} = \sum_{\substack{a,b,\\c,d}} \sigma(\varepsilon_b - \varepsilon_a) \delta_{\varepsilon_b - \varepsilon_a, \varepsilon_d - \varepsilon_c} J_x^{cb} \left(J_x^{ca}\right)^* L_{cd}^{\dagger} L_{ab}.$$
(4.33)

As a reminder, $\gamma(\varepsilon_b - \varepsilon_a) = \gamma(\omega) = J(\omega) (1 + n_b(\omega))$, with $n_b(\omega) = (e^{\omega\beta} - 1)^{-1}$ the Bose-Einstein distribution, and $J(\omega) = J_0 \omega e^{-\omega/\omega_c}$ was chosen to be parametrized by an ohmic spectral density. As the energy difference in $\gamma(\omega)$ can be positive, negative, or zero, the function can take three different forms,

$$\gamma(\omega) = \begin{cases} J(\omega) \left(1 + n_b(\omega)\right), & \omega > 0\\ J_0/\beta, & \omega = 0\\ J(|\omega|)n_b(|\omega|), & \omega < 0. \end{cases}$$
(4.34)

As the name of the Lamb-shift Hamiltonian already implies, it causes only a small shift in the energy levels and can thus be neglected. The final Lindblad master equation, which will be used later to describe the thermalization processes in this model is therefore

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}}(t) = -i\left[H_{\mathrm{S}},\rho_{\mathrm{S}}(t)\right] + \sum_{\substack{a,b,\\c,d}}\gamma_{ab,cd}\left(L_{ab}\rho_{\mathrm{S}}(t)L_{cd}^{\dagger} - \frac{1}{2}\left\{L_{cd}^{\dagger}L_{ab},\rho_{\mathrm{S}}(t)\right\}\right).$$
(4.35)

Note that because of $J_x^{ab} \ge 0$ for all a, b and $\gamma(\omega) > 0$ for all ω , it holds that $\gamma_{ab,cd} \ge 0$, which guarantees the positivity of $\rho_{s}(t)$.

4.1.5 Proving the KMS Condition

To show that the KMS condition holds for this model, it is necessary to show

$$\gamma(-\omega) = e^{-\beta\omega}\gamma(\omega). \tag{4.36}$$

As the Markov approximation was made under the assumption that the system is weakly coupled to the phononic bath, the KMS condition implies detailed balance, i.e. it would be sufficient to consider only the populations of $\rho_{\rm S}(t)$.

Claim: Above KMS condition (4.36) is true for this model.

Proof:

In order to show this relation, following identity is needed:

$$n_b(-\omega) = \frac{1}{e^{-\beta\omega} - 1} = \frac{e^{\beta\omega}}{1 - e^{\beta\omega}} = -e^{\beta\omega}\frac{1}{e^{\beta\omega} - 1} = -e^{\beta\omega}n_b(\omega).$$

For $\omega = 0$, the KMS condition becomes $\gamma(0) = \gamma(0)$, which is trivial. As for the case $\omega < 0$, it can be immediately brought into the form of the case where $\omega > 0$ by multiplying the KMS condition with $e^{-\beta\omega}$. This means, that it is sufficient to prove the case for $\omega > 0$.

Let $\omega > 0$. Setting up two equations:

$$\gamma(\omega) = J(\omega) \left(1 + n_b(\omega) \right) = J(\omega) + J(\omega)n_b(\omega).$$
(1)

It holds that $\gamma(-\omega) = J(\omega)n_b(\omega) = J(\omega)n_b(\omega) + J(\omega) - J(\omega) = -J(\omega) + J(\omega)(1 + n_b(\omega))$. Previously in the derivation of the Lindblad master equation it was shown that $n_b(-\omega) = -(1 + n_b(\omega))$. Using this and the relation in the beginning of this proof, one finds

$$\gamma(-\omega) = -J(\omega) + e^{\beta\omega}J(\omega)n_b(\omega).$$
(2)

Adding up (1) and (2) results in

$$\gamma(\omega) + \gamma(-\omega) = J(\omega) + J(\omega)n_b(\omega) - J(\omega) + e^{\beta\omega}J(\omega)n_b(\omega)$$

= $\underbrace{J(\omega)n_b(\omega)}_{=\gamma(-\omega)} + e^{\beta\omega}\underbrace{J(\omega)n_b(\omega)}_{=\gamma(-\omega)}$
= $\gamma(-\omega) + e^{\beta\omega}\gamma(-\omega).$

From this equation one obtains

$$\gamma(-\omega) = e^{-\beta\omega}\gamma(\omega).$$

4.2 Rate Equations

As the KMS condition is fulfilled for the interacting collective-spin model, it is sufficient to consider populations only. This means, it is necessary to derive a rate equation from the master equation (4.35), which describes how the diagonal entries of $\rho_{s}(t)$ evolve in time.

The operators L_{ab} and L_{cd}^{\dagger} can be written in any basis that diagonalizes $H_{\rm S}$, where each basis vector is represented with a collective state $|\varepsilon_m\rangle = |j,m\rangle$, where $m \in \{-j, -j+1, ..., j-1, j\}$. For simplicity, j will be omitted in this notation, since it does not change in time, i.e. each basis vector will be denoted as $|m\rangle$.

Because $H_S \propto J_z^2$, each eigenvalue except 0 is doubly degenerate. This can give rise to non-vanishing coherences over time, directly contradicting the KMS condition. To avoid this dilemma, a new basis is chosen, which is constructed by

$$|m^{\pm}\rangle = \frac{1}{\sqrt{2}} \left(|m\rangle \pm |-m\rangle \right). \tag{4.37}$$

Although this new basis takes care of the degeneracies, there is still the open question of how to handle $|m = 0\rangle$. This problem can be postponed for now, as this state only appears for integer j. This means there will be two rate equations, one for half-integer values of j, and one for integer values of j.

4.2.1 Rate Equation for Half Integer j

The new basis has two subspaces in which m only has values from m = 1/2 to m = j. The basis states are orthogonal and the subspaces have independent dynamics, i.e. there are no overlaps from one subspace to another, as following relations are true for all n, m,

$$\langle n^{\pm} | m^{\pm} \rangle = \delta_{n,m}, \tag{4.38}$$

$$\langle n^+ | m^- \rangle = 0, \tag{4.39}$$

$$\langle n^+ | J_z^2 | m^- \rangle = 0, \tag{4.40}$$

$$\langle n^+ | J_x | m^- \rangle = 0.$$
 (4.41)

These properties can be proven by direct computation. The rate equation can be found by determining $\langle n^{\pm} | \dot{\rho}_{\rm S}(t) | m^{\pm} \rangle =: \dot{\rho}_{n,m}$. Making use of the relations

$$H_{\rm S} \left| m^{\pm} \right\rangle = \lambda \omega_0 J_z^2 \left| m^{\pm} \right\rangle = \lambda \omega_0 m^2 \left| m^{\pm} \right\rangle, \tag{4.42}$$

$$J_x = \frac{1}{2} \left(J_+ + J_- \right), \tag{4.43}$$

$$J_{\pm} |m\rangle = \sqrt{j(j+1) - m(m\pm 1)} |m\pm 1\rangle = \alpha_m^{\pm} |m\pm 1\rangle, \qquad (4.44)$$

$$J_{\pm} |-m\rangle = \sqrt{j(j+1)} - m(m \mp 1) |-m \pm 1\rangle = \alpha_m^{\mp} |-m \pm 1\rangle, \qquad (4.45)$$

where

$$\alpha_m^{\pm} := \sqrt{j(j+1) - m(m\pm 1)} \tag{4.46}$$

was defined, the unitary evolution part of the master equation yields

$$\langle n^{\pm} | \left(-i \left[H_{\rm S}, \rho_{\rm S}(t) \right] \right) | m^{\pm} \rangle = -i\lambda\omega_0 (n^2 - m^2) \langle n^{\pm} | \rho_{\rm S}(t) | m^{\pm} \rangle = -i\lambda\omega_0 (n^2 - m^2)\rho_{n,m}, \qquad (4.47)$$

and $\gamma_{ab,cd}$ is found to be

$$\gamma_{ab,cd} = \frac{1}{4} \gamma(\varepsilon_b - \varepsilon_a) \delta_{\varepsilon_b - \varepsilon_a, \varepsilon_d - \varepsilon_c} \left(\alpha_b^+ \alpha_d^+ \delta_{a,b+1} \delta_{c,d+1} + \alpha_b^- \alpha_d^- (\delta_{a,b-1} \delta_{c,d-1} + \delta_{a,b} \delta_{b,1/2} \delta_{c,d} \delta_{d,1/2}) \right).$$
(4.48)

The non-unitary part of the master equation is more tedious to find and requires additionally the usage of

$$\alpha_{-m}^{\pm} = \alpha_m^{\mp}, \tag{4.49}$$

$$\alpha_{m+1}^- = \alpha_m^+,\tag{4.50}$$

$$\alpha_{m-1}^{+} = \alpha_{m}^{-}.$$
 (4.51)

These relations can be proven directly by checking the respective Clebsch-Gordan coefficients. As there are three summands in $\gamma_{ab,cd}$, there are a total of nine sums to evaluate. Since they are all done in a similar way, only one is demonstrated here as an example.

Considering the first sum in

$$\sum_{\substack{a,b,\\c,d}} \gamma_{ab,cd} \left(L_{ab} \rho_{\rm S}(t) L_{cd}^{\dagger} - \frac{1}{2} \left\{ L_{cd}^{\dagger} L_{ab}, \rho_{\rm S}(t) \right\} \right), \tag{4.52}$$

one finds

$$\sum_{\substack{a,b,\\c,d}} \frac{1}{4} \gamma(\varepsilon_b - \varepsilon_a) \delta_{\varepsilon_b - \varepsilon_a, \varepsilon_d - \varepsilon_c} \alpha_b^+ \alpha_d^+ \delta_{a,b+1} \delta_{c,d+1} \delta_{n,a} \delta_{c,m} \langle b^\pm | \rho_{\rm S}(t) | d^\pm \rangle$$

$$= \frac{1}{4} \gamma(\varepsilon_{n-1} - \varepsilon_n) \delta_{\varepsilon_{n-1} - \varepsilon_n, \varepsilon_{m-1} - \varepsilon_m} \alpha_{n-1}^+ \alpha_{m-1}^+ \langle (n-1)^\pm | \rho_{\rm S}(t) | (m-1)^\pm \rangle$$

$$= \frac{1}{4} \delta_{n,m} \gamma(\varepsilon_{n-1} - \varepsilon_n) \alpha_n^- \alpha_m^- \rho_{n-1,m-1}.$$
(4.53)

The last Kronecker delta was deliberately not evaluated yet, because it vanishes for coherences.

Collecting all terms, the general rate equation is identical for both subspaces, and is given for half-integer values of j by

$$\begin{split} \dot{\rho}_{n,m} &= -i\lambda\omega_{0}(n^{2} - m^{2})\rho_{n,m} \\ &+ \frac{1}{4}\delta_{n,m}\gamma(\varepsilon_{n-1} - \varepsilon_{n})\alpha_{n}^{-}\alpha_{m}^{-}\rho_{n-1,m-1} \\ &+ \frac{1}{4}\delta_{n,m}\gamma(\varepsilon_{n+1} - \varepsilon_{n})\alpha_{n}^{+}\alpha_{m}^{+}\rho_{n+1,m+1} \\ &+ \frac{1}{4}\delta_{n,m}\delta_{m,1/2}\gamma(0)\left(\alpha_{1/2}^{-}\right)^{2}\rho_{n,m} \\ &- \frac{1}{8}\gamma(\varepsilon_{n} - \varepsilon_{n+1})\left(\alpha_{n}^{+}\right)^{2}\rho_{n,m} \\ &- \frac{1}{8}\gamma(\varepsilon_{n} - \varepsilon_{n-1})\left(\alpha_{n}^{-}\right)^{2}\rho_{n,m} \\ &- \frac{1}{8}\delta_{n,1/2}\gamma(0)\left(\alpha_{1/2}^{-}\right)^{2}\rho_{n,m} \\ &- \frac{1}{8}\gamma(\varepsilon_{m} - \varepsilon_{m+1})\left(\alpha_{m}^{+}\right)^{2}\rho_{n,m} \\ &- \frac{1}{8}\gamma(\varepsilon_{m} - \varepsilon_{m-1})\left(\alpha_{m}^{-}\right)^{2}\rho_{n,m} \\ &- \frac{1}{8}\delta_{m,1/2}\gamma(0)\left(\alpha_{1/2}^{-}\right)^{2}\rho_{n,m} . \end{split}$$
(4.54)

Taking a look at the coherences, where $n \neq m$, the rate equation simplifies to a single uncoupled ordinary differential equation for $\rho_{n,m}$. Because it is possible to factorize an overall minus sign on all summands on the right-hand side, the solution is proportional to a decaying exponential function. This confirms what was said earlier, namely that all coherences vanish over time.

For the populations, where n = m, the rate equation simplifies considerably to

$$\dot{\rho}_{m,m} = \frac{1}{4} \gamma(\varepsilon_{m-1} - \varepsilon_m) \left(\alpha_m^-\right)^2 \rho_{m-1,m-1} + \frac{1}{4} \gamma(\varepsilon_{m+1} - \varepsilon_m) \left(\alpha_m^+\right)^2 \rho_{m+1,m+1} - \frac{1}{4} \gamma(\varepsilon_m - \varepsilon_{m-1}) \left(\alpha_m^-\right)^2 \rho_{m,m} - \frac{1}{4} \gamma(\varepsilon_m - \varepsilon_{m+1}) \left(\alpha_m^+\right)^2 \rho_{m,m}.$$

$$(4.55)$$

Note that for m = 1/2 the first row cancels with the third row due to $\varepsilon_{-m} = \varepsilon_m$ for all m, and

$$\langle m - 1^{\pm} | \rho | m - 1^{\pm} \rangle \Big|_{m=1/2} = \langle -1/2^{\pm} | \rho | -1/2^{\pm} \rangle = \frac{1}{2} \left(\langle -1/2 | \pm \langle 1/2 | \right) \rho \left(| -1/2 \rangle \pm | 1/2 \rangle \right)$$

$$= \frac{1}{2} \left(\langle 1/2 | \pm \langle -1/2 | \right) \rho \left(| 1/2 \rangle \pm | -1/2 \rangle \right) = \langle 1/2^{\pm} | \rho | 1/2^{\pm} \rangle$$

$$= \rho_{1/2,1/2}.$$

$$(4.56)$$

Thus, for m = 1/2 equation (4.55) can be written as

$$\dot{\rho}_{1/2,1/2} = \frac{1}{4} \gamma(\varepsilon_{3/2} - \varepsilon_{1/2}) \left(\alpha_{1/2}^+\right)^2 \rho_{3/2,3/2} - \frac{1}{4} \gamma(\varepsilon_{1/2} - \varepsilon_{3/2}) \left(\alpha_{1/2}^+\right)^2 \rho_{1/2,1/2}.$$
(4.57)

4.2.2 Rate Equation for Integer j

For all systems with an integer value for j there is an eigenvalue of 0, which is not degenerate. This means that one of the subspaces needs to be extended with the $|m = 0\rangle$ state. Using equation (4.37) with $|m = 0\rangle$ results in a non-zero value for the +-subspace only, expressed as

$$\frac{1}{\sqrt{2}}\left(\left|0\right\rangle + \left|0\right\rangle\right) = \sqrt{2}\left|0\right\rangle =: \left|0^{+}\right\rangle.$$
(4.58)

With this, the +-subspace consists of the set $\{ \{|m^+\rangle\}, \sqrt{2} |0\rangle \}$ for $m \in \{1, ..., j\}$, whereas the other subspace only contains $\{ \{|m^-\rangle\} \}$ for the same m. Because the integer case describes the same system as the half-integer case, a very similar rate equation is expected, with the only difference being around the zero state. There is also no need to get a rate equation for each subspace because of the symmetry of the two for m > 0. This means that it is sufficient to consider only the +-subspace to find a rate equation, since all entries of the system's density matrix for m > 0 are by symmetry the same as in the other subspace.

As in the half-integer case, the two subspaces are orthogonal and show independent dynamics, i.e. for all n, m it holds that

$$\langle n^{\pm} | m^{\pm} \rangle = \delta_{n,m}, \tag{4.59}$$

$$\langle n^+ | m^- \rangle = 0, \tag{4.60}$$

$$\langle n^+ | J_z^2 | m^- \rangle = 0,$$
 (4.61)

$$\langle n^+ | J_x | m^- \rangle = 0. \tag{4.62}$$

All these relations can be proven by direct computation. Since the approach to find the rate equation is equal to the half-integer case, there is no need to sketch out the derivation again. Instead, the solution is presented directly. Hence, the general rate equation is given by

$$\begin{split} \dot{\rho}_{n,m} &= -i\lambda\omega_{0}(n^{2} - m^{2})\rho_{n,m} \\ &+ \frac{1}{4} \left[\delta_{n,m}\gamma(\varepsilon_{n-1} - \varepsilon_{n})\alpha_{n}^{-}\alpha_{m}^{-}\rho_{n-1,m-1} \right]_{(n,m>0)} \\ &+ \frac{1}{4} \left[\delta_{n,m}\gamma(\varepsilon_{n+1} - \varepsilon_{n})\alpha_{n}^{+}\alpha_{m}^{+}\rho_{n+1,m+1} \right]_{(n,m>0)} \\ &+ \frac{1}{2}\delta_{n,m}\delta_{m,0}\gamma(\varepsilon_{1} - \varepsilon_{0}) (\alpha_{0})^{2} \rho_{1,1} \\ &- \frac{1}{8} \left[\gamma(\varepsilon_{n} - \varepsilon_{n+1}) (\alpha_{n}^{+})^{2} \rho_{n,m} \right]_{(n>0)} \\ &- \frac{1}{8} \left[\gamma(\varepsilon_{n} - \varepsilon_{n-1}) (\alpha_{n}^{-})^{2} \rho_{n,m} \right]_{(n>0)} \\ &- \frac{1}{4}\delta_{n,0}\gamma(\varepsilon_{0} - \varepsilon_{1}) (\alpha_{0})^{2} \rho_{n,m} \\ &- \frac{1}{8} \left[\gamma(\varepsilon_{m} - \varepsilon_{m+1}) (\alpha_{m}^{+})^{2} \rho_{n,m} \right]_{(m>0)} \\ &- \frac{1}{8} \left[\gamma(\varepsilon_{m} - \varepsilon_{m-1}) (\alpha_{m}^{-})^{2} \rho_{n,m} \right]_{(m>0)} \\ &- \frac{1}{4}\delta_{m,0}\gamma(\varepsilon_{0} - \varepsilon_{1}) (\alpha_{0})^{2} \rho_{n,m} . \end{split}$$

$$(4.63)$$

Just as expected, an overall minus sign for the coherences $(n \neq m)$ can be factorized, so that the rate equation for each non-diagonal entry in the density matrix reduces to a single uncoupled ordinary differential equation. Albeit some oscillating part in its solution, it is still proportional to a decaying exponential function, leading to the expected vanishing of all coherences over time.

For the populations, the rate equation simplifies to

$$\dot{\rho}_{m,m} = \frac{1}{4} \left[\gamma(\varepsilon_{m-1} - \varepsilon_m) \left(\alpha_m^{-} \right)^2 \rho_{m-1,m-1} \right]_{(m>0)} \\ + \frac{1}{4} \left[\gamma(\varepsilon_{m+1} - \varepsilon_m) \left(\alpha_m^{+} \right)^2 \rho_{m+1,m+1} \right]_{(m>0)} \\ - \frac{1}{4} \left[\gamma(\varepsilon_m - \varepsilon_{m-1}) \left(\alpha_m^{-} \right)^2 \rho_{m,m} \right]_{(m>0)} \\ - \frac{1}{4} \left[\gamma(\varepsilon_m - \varepsilon_{m+1}) \left(\alpha_m^{+} \right)^2 \rho_{m,m} \right]_{(m>0)} \\ + \frac{1}{2} \delta_{m,0} \gamma(\varepsilon_1 - \varepsilon_0) \left(\alpha_0 \right)^2 \rho_{1,1} \\ - \frac{1}{2} \delta_{m,0} \gamma(\varepsilon_0 - \varepsilon_1) \left(\alpha_0 \right)^2 \rho_{0,0}.$$

$$(4.64)$$

as soon as m > 0, this rate equation takes the same form as in the half-integer case. This is expected, since, as mentioned previously, both rate equations describe the same system.

Both rate equations imply a superradiant behaviour, as all Clebsch-Gordan coefficients appear squared. This leads to a scaling proportional to j^2 and hence, N^2 if $m \approx 0$. Thus, there is a similar behaviour as in the non-interacting collective-spin model. The dissipation factors γ are not constant anymore, but functions of energy differences. This takes care of the quadratic scaling in the energy differences of the energy levels, which were equidistant in the linear model.

4.3 Testing the Rate Equations

Because the fully thermalized states are Gibbs states, their analytical expression is known. As in the linear model, this can be used to test, whether the rate equations (4.55) and (4.64) thermalize an initial state towards the correct fully thermalized Gibbs state. Here, analogous to Section 3.2, the quantum relative entropy was used as a measure of closeness. As the initial state gets closer to the fully thermalized state, the quantum relative entropy is expected to decay to zero over time. For each rate equation the scenarios of heating the system up and of cooling it down were tested. The results are shown in Figure 4.2. For all settings the temperature of the cold heat bath was set to $T_c = \omega_0$, and the temperature of the hot heat bath was set respectively to $T_h = 8\omega_0$. The dimensionless control parameter was set to $\lambda_f = 3$ for heating the system up, and $\lambda_i = 1$ for cooling it down. Lastly, for the integer case j = 1 was chosen, and j = 3/2 for the half-integer case. All plots in Figure 4.2 exhibit the expected behaviour, thus justifying the usage of the rate equations.





Figure 4.2: Quantum relative entropy over time. The red lines correspond to heating the working fluid up, where as the blue lines depict a cooling down. The parameters are set to $T_c = \omega_0$, $T_h = 8\omega_0$, $\lambda_i = 1$, $\lambda_f = 3$. For (a) and (b) is j = 1, and for (c) and (d) is j = 3/2.

4.4 Employing the Quantum Otto Cycle

Using the interacting collective-spin model as a working fluid in the quantum Otto cycle, the thermal strokes can be described with the previously derived Lindblad master equation (4.35). The unitary strokes can be represented as in the non-interacting collective-spin model, i.e. they can be done with

$$1 \longrightarrow 2: \quad T_c \mapsto T'_c = \frac{\lambda_f}{\lambda_i} T_c,$$

$$3 \longrightarrow 4: \quad T_h \mapsto T'_h = \frac{\lambda_i}{\lambda_f} T_h.$$
(4.65)

As for the efficiency of a converged cycle, it also stays the same as in the linear model, namely

$$\eta = 1 + \frac{Q_c}{Q_h} = 1 + \frac{\operatorname{Tr}\left(H_i(\rho_3 - \rho_1)\right)}{\operatorname{Tr}\left(H_f(\rho_1 - \rho_3)\right)} = 1 + \frac{\operatorname{Tr}\left(\lambda_i\omega_0 J_z^2(\rho_3 - \rho_1)\right)}{\operatorname{Tr}\left(\lambda_f\omega_0 J_z^2(\rho_1 - \rho_3)\right)}$$
$$= 1 - \frac{\lambda_i}{\lambda_f} \frac{\operatorname{Tr}\left(\omega_0 J_z^2(\rho_1 - \rho_3)\right)}{\operatorname{Tr}\left(\omega_0 J_z^2(\rho_1 - \rho_3)\right)} = 1 - \frac{\lambda_i}{\lambda_f}.$$

As in the linear model, the quadratic model behaves similarly in the sense, that when the coupling time is smaller than the time needed for a full thermalization, the heat machine goes into a converged cycle. This is visualized in Figure 4.3, where the quantum Otto cycle was employed with j = 7/2, $\lambda_i = 1$, $\lambda_f = 3$, $T_c = 10\omega_0$, and $T_h = 80\omega_0$. In Figure 4.3a, each thermal stroke was long enough for a full thermalization. The circled numbers represent the positions during the cycle as labelled in Figure 3.1. In Figure 4.3b, the coupling time was set sufficiently small, such that no full thermalization occurred. The converged cycle is indicated in red. As long as all parameters are not perturbed, the heat engine stays within this converged cycle.

Similar to the non-interacting collective-spin model, the thermalization time is expected to be dependent on the number of two-level systems in the working fluid, and hence on j. Since each rate equation consists of a set of coupled linear differential equations, it is in principal possible to find an analytical solution for every value of j. But as the number of coupled differential equations is also proportional to j, it is reasonable to do a numerical calculation to find how the thermalization time is dependent on j. Therefore, the thermal baths are set to have temperatures of $T_c = \omega_0$, and $T_h = 4\omega_0$. The control parameters were set to $\lambda_i = 1$ and $\lambda_f = 3$. As in the linear model, the initial state is chosen to be in thermal equilibrium with the hot heat bath and cooled down until a thermal equilibrium with the cold heat bath is reached. The resulting thermalization times are shown in Figure 4.4.



Figure 4.3: (a): Quantum Otto cycle with full thermalization during the thermal strokes. The circled numbers represent the positions in the cycle as depicted in Figure 3.1. (b): The dashed line represents the cycle with full thermalization as shown in (a). The black solid lines show the cycles that were necessary to reach the converged cycle, which is highlighted in red. The coupling time was chosen to be $t\omega_0 = 0.02$.



Figure 4.4: Dependence of the thermalization time on j. The heat engine was initialized with $T_h = 4\omega_0$, $T_c = \omega_0$, $\lambda_i = 1$, and $\lambda_f = 3$. A fit curve is added to show the thermalization time's proportionality to $1/j^2$.

According to Figure 4.4, the thermalization time is proportional to $1/j^2$. This dependence shows that the more two-level systems there are, the shorter are the thermalization times. This is expected, since the energy levels in the system are, compared to the non-interacting collective-spin model, no longer equidistantly distributed. Instead, the energy differences increase quadratically and hence, the occupation probabilities decrease faster for higher energy levels than in the linear model, as there is much more energy needed to occupy them.

Since the thermalization time in the quadratic model decreases faster with increasing j than in the linear model, a stronger superradiant effect is observed in Figure 4.5. This is due to the different energy differences between their energy levels in the collective eigenstates. They are generally larger than in the linear model, leading to smaller occupation probabilities for higher energy levels. This implies that it is more likely to occupy the regime around $m \approx 0$, giving rise to superradiance.

The superradiant effect can be seen better in Figure 4.5, where the power ouput of the heat engine is plotted over j for different temperatures of the hot heat bath, while the cold heat bath was always set to $T_c = \omega_0$. As usual, the dimensionless control parameters were arbitrarily chosen as $\lambda_i = 1$, and $\lambda_f = 3$. For the coupling time the same time scale was used as in Figure 3.5, $t\omega_0 = 1$. The power has a quadratic scaling around small values of j, indicated by the quadratic fit, and saturates for larger j. The saturation stems from the fact, that there is a finite power per converged cycle, even in the limit $j \longrightarrow \infty$. This can be explained with the same reasoning as in the non-interacting collective-spin model. But since the energy differences between two neighbouring energy levels increase quadratically for higher values of m, the corresponding occupation probabilities become lower faster than in the linear model. This explains why the maximal power output for a specific temperature in the heat bath is lower than in the non-interacting collective-spin model.



Figure 4.5: Power of the heat engine as a function of j. For each temperature of the hot heat bath were the remaining parameters set to $T_c = \omega_0$, $\lambda_i = 1$, and $\lambda_f = 3$. The coupling time is fixed to $t\omega_0 = 1$. A quadratic fit curve is added for $j \leq 5$ to show the quadratic scaling for small values of j, implying a superradiant effect.

Plotting the power output per converged cycle dependent on the coupling time, where $T_c = \omega_0$, $T_h = 8\omega_0$, $\lambda_i = 1$, and $\lambda_f = 3$ for different values of j, leads to Figure 4.6. As one can see, there is a finite power in the thermodynamic limit $j \rightarrow \infty$. It is also evident that in this setting even relatively small values of j are already close to the thermodynamic limit. Naturally small coupling times result in higher powers. But as soon as the time scale for full thermalization is reached, no further power can be extracted and a decrease in power occurs. The black dotted line indicates the coupling time used to create Figure 4.5.



Figure 4.6: Power of the collective-spin heat engine as a function of coupling time for different values of j. The dotted vertical line depicts the used coupling time for Figure 4.5, to which all parameters are set accordingly.

For the limit case $j \longrightarrow \infty$ no analytical expression has been found. Instead, the thermodynamic limit in Figure 4.6 was determined numerically.

5 Comparison of the Models

To make a comparison between the non-interacting collective-spin model and the interacting collectivespin model, it is necessary to initialize similar settings. For all plots above the dimensionless control parameters always were always the same. For the plots showing the thermalization time and the power the temperatures of the heat baths were the same, although additional temperatures of the hot reservoir have been used in Figure 4.5. Only on the plots where the whole quantum cycle is depicted, different temperatures were used for each heat bath, as well as different coupling times. This was done intentionally as with the same choice of these parameters Figure 4.3 does not give a good resolution of all operating cycles.

To get an appropriate comparison of the operating cycles between the linear and the quadratic model, both were initialized such that they have the same absolute mean energy. The second condition is that after the first unitary stroke, the same amount of work is invested in both cases. Thus, for a certain pair of λ_i and λ_f of the linear model a respective pair of $\tilde{\lambda}_i$ and $\tilde{\lambda}_f$ for the quadratic model can be numerically found. For a better understanding how exactly the two models were compared to each other, an exemplary plot in the style of Figure 3.3 and Figure 4.3 is given in Figure 5.1. For this example, the parameters were arbitrarily chosen to be j = 11/2, $T_c = 10\omega_0$, and $T_h = 40\omega_0$. Here, as well as for all calculations below, the finite coupling time for both models was set to $t\omega_0 = 0.1$. For this example, as well as for all further calculations, the dissipation rate for the non-interacting collective-spin model was set to $\gamma = 0.1\omega_0$. As for the dimensionless control parameters, they were chosen for the linear model to be the same as previously, $\lambda_i = 1$, and $\lambda_f = 3$.



Figure 5.1: Example of a setup to compare both discussed models. Both heat engines are initialized with the same absolute energy and bridge the same energy difference after the first unitary stroke. Like in Figure 3.3 and 4.3, the dashed lines represent the full thermalization cycles. The colored cycles stand for the converged cycles, red for the linear model, and blue for the quadratic model. All black cycles are necessary to reach the converged ones.

The joint parameters are set to $T_c = 10\omega_0$, $T_h = 40\omega_0$, $t\omega_0 = 0.1$, j = 11/2. The model-specific parameters for the linear model are $\gamma = 0.1\omega_0$, $\lambda_i = 1$, $\lambda_f = 3$, whereas for the quadratic model, it was numerically determined that $\tilde{\lambda}_i \approx 0.11$ and $\tilde{\lambda}_f \approx 0.32$.

In the linear model, the mean energies of the initialized heat engine are dependent on the eigenvalues of the collective-spin operator J_z . Thus, the calculated dimensionless control parameters for the interacting collective-spin model must be adjusted for each value of j. Moreover, it is only possible to determine the respective parameters up to the value of j, where the power according to Figure 4.5 begins to saturate. For larger j, no suitable values that match the imposed initial conditions can be found. There were three different settings with respect to the temperatures of the heat baths considered. The first one set $T_c = 5\omega_0$ and $T_h = 20\omega_0$, the second $T_c = 10\omega_0$ and $T_h = 40\omega_0$, and the third $T_c = 20\omega_0$ and $T_h = 80\omega_0$. The dimensionless control parameters for the linear model were the same for all calculations, namely $\lambda_i = 1$, and $\lambda_f = 3$. Because of the constraint that fitting control parameters for the quadratic model can only be found up to a specific j, each plot in Figure 5.2 has a different range of j depicted. Generally, the determined control parameters need to increase with growing system size. However, they can be approximated to be constant with a sufficiently large temperature of the hot heat bath.



Figure 5.2: Dimensionless control parameters $\tilde{\lambda}_i$ and $\tilde{\lambda}_f$ as functions of j for the quadratic model. The coupling time is fixed for all j to $t\omega_0 = 0.1$.

Using the depicted parameters in Figure 5.2, the corresponding temperatures for the heat baths, and all other parameters as used above in the example for Figure 5.1, the power outputs of the respective converged cycles were numerically determined and plotted in Figure 5.3.



Figure 5.3: Power of the converged cycle dependent on j for both discussed models. The red dots depict the powers for the non-interacting collective-spin model, and the blue dots show the powers for the interacting collective-spin model. The chosen temperatures of the respective heat baths are denoted under each plot.

The power outputs of the non-interacting collective-spin model are very similar for all depicted temperatures. This is because the range of j is not big enough. Since each temperature of the hot heat bath leads to a different maximally possible power output, differences would appear similarly as in Figure 3.5 for sufficiently large j. The powers of the quadratic model however show very different values depending on T_h . For small j, the linear model is more favourable in terms of power. Additionally the maximally possible work that can be extracted is generally higher than for the quadratic model. Even though it is not possible to find fitting control parameters that match the desired initial conditions from a specific j on, Figure 5.3 indicates that there are settings for which the interacting collective-spin model outperforms the non-interacting collective-spin model. However, these settings can only be realized in a specific interval of j, due to the higher maximally possible power in the linear model mentioned before. Thus, for the interacting collective-spin model to be more beneficial, some fine tuning of all parameters is necessary.

6 Discussion

In the following section it is checked if all the assumptions made in the derivation for the Lindblad master equation are valid.

6.1 Validity of the Master Equation for the Interacting Collective Spin Model

There were three assumptions made in the derivation of the master equation. The first led to the Born approximation and required the heat baths to be much larger than the system. This assumption can be seen as fulfilled, as the upper bound of the sum in the bath Hamiltonian (4.2) can be taken arbitrarily large. The second one allowed the Markov approximation and imposed a weak coupling and a rapidly decaying bath correlation time, compared to the relaxation time of the system. The parameter responsible for the collective coupling to the bath is the dimensionless coupling constant J_0 , which was set to $J_0 = 1$ in all calculations, ensuring the weak coupling. As for the time scales, the bath-correlation function (4.22) gives a complex number as an output value. By using $|z| \ge \operatorname{Re}(z)$ and $|z| \ge \operatorname{Im}(z)$ for all $z \in \mathbb{C}$, it is possible to find an upper bound for the bath-correlation time τ_{B} . Choosing a small tolerance value $\varepsilon > 0$, for which it holds that

$$\left| \langle \hat{B}(\tau_{\rm B}) \hat{B}(0) \rangle \right| = \varepsilon, \tag{6.1}$$

and solving for $\tau_{\rm B}$ yields

$$\tau_{\rm B} = \frac{1}{2\pi T} \operatorname{arcosh}\left(\frac{J_0 \pi T^2}{\varepsilon} + \cos\left(\frac{2\pi T}{\omega_c}\right)\right) \approx \frac{1}{2\pi T} \operatorname{arcosh}\left(\frac{J_0 \pi T^2}{\varepsilon}\right).$$
(6.2)

The last approximation is justified because of $J_0 \pi T^2 / \varepsilon \gg 1$. The expression for the bath-correlation time scale diverges as ε goes to zero. That is the reason why this tolerance value was introduced. It can be chosen small enough such that all correlations within the bath are negligible. The relaxation time $\tau_{\rm R}$ can be identified with the thermalization time. It was obtained numerically, since an analytical expression requires an analytical solution for the rate equations (4.55) and (4.64).

The third important assumption to be considered is the secular approximation, in which rapidly oscillating terms are neglected. Thus, the evolution time $\tau_{\rm S}$ for the working fluid needs to be much smaller than the relaxation time. The former is dependent on the differences of eigenenergies of the system's Hamiltonian. Therefore, this time scale can be expressed as

$$\tau_{\rm S} := \max_{\omega \neq \omega'} \frac{1}{|\omega - \omega'|} = \frac{1}{2\lambda\omega_0} \tag{6.3}$$

To be consistent with the Markov approximation, the time scale τ_S needs to be smaller than the bath-correlation time, so that

$$\tau_{\rm S} < \tau_{\rm B} \ll \tau_{\rm R}.\tag{6.4}$$

The first inequality in (6.4) holds, since all variables, that appear in τ_S do not influence τ_B and vice versa. Hence there is no violation of the relation between these two time scales even for small non-trivial systems, as long as the temperature of the reservoirs are chosen to be sufficiently small, or equivalently, as long as λ is chosen sufficiently large. Because there is no analytical expression for τ_R , only numerical tests can be done. Therefore, a couple of different scenarios have been considered to create some plots that show all three time scales over j.

To be able to make a reasonable statement, the dimensionless parameters were set to $\lambda_i = 1$, and $\lambda_f = 3$. For all these plots different temperatures of the heat baths were chosen. For consistency, the working fluid was always once initialized to be in thermal equilibrium with the cold heat bath and then coupled to the hot heat bath, until the new thermal equilibrium was reached, and vice versa. All resulting plots are shown in Figure 6.1.



Figure 6.1: Thermalization time $\tau_{\rm R}$, bath-correlation time $\tau_{\rm B}$, and the time scale for the evolution of the system $\tau_{\rm S}$ for different temperature settings of the heat baths, as denoted under each plot. The control parameters are set to $\lambda_i = 1$, and $\lambda_f = 3$. Thermalizations that correspond to the cooling of a system are denoted with a 'C', whereas thermalizations that correspond to heating a system are denoted with an 'H'.

The inequalities in equation (6.4) need to be true if no assumptions made for the Lindblad master equation are violated. The plots in Figure 6.1 clearly indicate that there is only a very limited regime of parameter choices that are valid under all assumptions. Moreover, these plots suggest that the assumptions hold for small temperatures of the heat baths and small values of j. For larger temperatures the relaxation time $\tau_{\rm R}$ becomes too small, such that $\tau_{\rm S}$ is greater than $\tau_{\rm R}$ for all possible system sizes. Because of the temperature dependence of the bath-correlation time, there are settings, where $\tau_{\rm B} > \tau_{\rm S}$ for small j, which violate the conditions of the secular approximation. This means that in order to have no violations at all, there is always some fine tuning of all involved parameters necessary.

In summary, the Lindblad master equation (4.35) is applicable for sufficiently small j and low temperatures to provide some meaningful insight. However, for larger j or higher temperatures, different approaches should be used, e.g. one could use a Redfield master equation instead of the Lindbladian form. However, Redfield equations generally do not guarantee the positivity of density matrices in their time evolution [30,31]. Hence, this method can potentially be problematic. Another possibility would be a 'coarse-graining' approach, which does also not rely on the secular approximation [41], or one could use the recently developed method of a thermofield-based chain mapping for open quantum systems to avoid the secular approximation and its restrictions [42]. Nevertheless, the results in Section 4 do not indicate a violation of any of the assumptions. Moreover, the results confirm the expectation that a superradiant effect can be numerically observed. Thus, to study superradiance in a quantum heat engine, the approach in this work seems feasible.

6.2 Superradiant Effect and Power

The superradiant effect in the interacting collective-spin model can be observed in several instances. It is already visible in the rate equations (4.55) and (4.64). The Clebsch-Gordan coefficients exhibit a proportionality of j^2 (and hence of N^2) for eigenstates where m = 0, which is typical for superradiance. This proportionality exists only for these eigenstates. But since the Clebsch-Gordan coefficients around $m \approx \pm j$ are much smaller than around $m \approx 0$ for $j \gg 1$, there is still some superradiant scaling for the latter coefficients.

The Lindblad master equation (4.35) describes the changes in the occupation-probability distribution dependent on the energy gaps in the working fluid's collective energy levels. Because these are quadratically spaced, the energy gaps around the higher energy levels are much bigger than around the collective ground state. This has direct consequences for the changes in the populations when the collective-spin model is employed in the quantum Otto cycle. Systems with a higher j are faster fully thermalized than smaller ones and the respective power output per converged cycle shows a superradiant scaling for small j, before saturating to a maximal possible value.

In comparison with the linear model the superradiant scaling appears to be more visible in the quadratic model. This is due to the different gap sizes between the energy levels in the two models. In the former model the energy gaps are all equal in size, leading to a faster flattening of the quadratic scaling than in the latter model. However, although the superradiant effect in the non-interacting collective-spin model is not as strong as in the interacting collective-spin model, the maximal possible power output per converged cycle for the same choices of control parameters, temperatures, and coupling time is greater than in the quadratic model.

When both models are initialized with the same absolute energy and bridge the same energy difference after the first unitary stroke, then there are some settings for which the quadratic model outperforms the linear model. Since this requires some fine tuning of all involved parameters the non-interacting collective-spin model is more practicable, due to generally having a larger maximal possible work extraction per cycle. However, if one wants to demonstrate the superradiant effect, the interacting collective-spin model is more suitable. In regard to superradiance, the quadratic scaling of the power output is clearly more evident for the quadratic model in Figure 5.3, especially for lower temperatures. For the case where $T_h = 80\omega_0$ the range of j is too small to draw a conclusion. But considering Figure 4.5, a superradiant effect can be expected nevertheless.

7 Conclusion

In this work, two different models for a working fluid employed in a quantum Otto cycle have been studied. The focus was laid on their respective superradiant scaling in the power output per converged cycle.

The results for the non-interacting collective-spin model were presented by Kloc, Cejnar, and Schaller [26] in 2019. These findings can be confirmed, as all results presented in this thesis agree with the earlier work. Based on them the hypothesis was formed that the superradiant scaling in the power output with the size of the system should be easily observed even for small temperatures, because the collective ground state in this model already has the large Clebsch-Gordan coefficients. To test this hypothesis, a Lindblad master equation has been derived, based on the Born-Markov and secular approximations. This Lindbladian was then used to describe the thermal strokes in the quantum Otto cycle.

It has been found in this thesis that the superradiant scaling can be numerically observed even for small temperatures and that it is more pronounced in the interacting collective-spin model. But although the superradiant effect is stronger, the power output is generally smaller than in the non-interacting collective-spin model. Therefore, even though there are settings for which the quadratic model outperforms the linear model, in terms of power it is more practicable to employ a non-interacting collective-spin model as a working fluid.

It was also tested, whether the assumptions made during the microscopic derivation of the master equation were violated. It was found, that for small temperatures in the heat baths and small values of j, the assumptions hold, but for higher temperatures the secular approximation is violated. Because there is no indication of this in the results shown earlier, it is suggested to make another approach, that does not rely on the secular approximation, to recalculate the findings. A possibility would be to use a Redfield master equation, a coarse-graining method, or a thermofield-based chain mapping for open quantum systems.

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Appendix

A. Superradiance

In 1954, R. Dicke published a paper in which he coined the term superradiance [43]. He investigated a system of N two-level atoms, all prepared in the excited state and confined in a cavity smaller than the wavelength of a photon emitted by an atom during its decay to its ground state. The maximally excited system is able to revert to its collective ground state by a 'chain reaction' of all N decaying twolevel atoms, induced by an initially spontaneously emitted photon. Because of the small confinement, the emitted photons are indistinguishable and interfere constructively. Through this emission process, an electromagnetic field emerges with an energy density proportional to N^2 . This form of coherent emission has been labelled 'collective spontaneous emission' or 'Dicke superradiance' [44]. It stands in contrast to the incoherent emission, where the emission energy density is proportional to N (see Figure A.1) [45, 46].



Figure A.1: Upper image: Incoherent emission of all N atoms. The emission intensity decays exponentially over time τ_{Sp} . Lower image: Coherent emission of the atoms leading to a transient peak in the emission energy. Figure taken from [46].

According to Gross and Haroche [46], the superradiant emission can be compared to an 'ordering' of atomic dipole moments. Before the first emission of a photon in the atomic gas takes place, there is no optical dipole in the medium. After the first emission however, an electromagnetic field emerges which causes even more dipoles to appear. The eventual appearance of dipole–dipole correlations leads to the chain reaction described above.

To describe collective states, a formalism involving collective operators is used. Following Gross and Haroche [46], suppose that each atomic two-level system has a ground state denoted as $|0\rangle$ and an excited state denoted as $|1\rangle$. Transitions of one energy level to the other can be described by introducing raising and lowering operators D_i^{\pm} defined as

$$D_i^+ = |1\rangle \langle 0|; \quad D_i^- = |0\rangle \langle 1|.$$
 (A.1)

Moreover, the diagonal operator D_i^3 can be defined as

$$D_i^3 = \frac{1}{2} \left(\left| 1 \right\rangle \left\langle 1 \right| - \left| 0 \right\rangle \left\langle 0 \right| \right). \tag{A.2}$$

The index i indicates that they act only on the ith atomic subspace. They obey the same commutation relations as the spin-1/2 Pauli operators, namely

$$\left[D_i^3, D_j^{\pm}\right] = \pm \delta_{ij} D_i^{\pm}; \quad \left[D_i^+, D_j^-\right] = 2\delta_{ij} D_i^3. \tag{A.3}$$

If all particles are in their excited state, then the total state of the whole system at time t = 0 can be written as $|\Psi(0)\rangle = |1, 1, ..., 1\rangle$. Now, two assumptions are needed. The first assumption is that the evolution of this state is only influenced by the coupling of the atoms to the radiation field. All other interactions like e.g. collisions are neglected. The second assumption is that the coupling is symmetrical with respect to the exchange of any two atoms in the system. With these assumptions the coupling between the atomic states and the radiating field is invariant under atomic permutations.

For a convenient description of the collective states, each two-level atom can be considered as a fictitious spin-1/2 system, where the excited state corresponds to the spin up and the ground state to the spin down state. Since the previously defined operators reveal analogous properties when acting on an atomic state, they can be mapped to the Pauli operators. Because each N-atom state is invariant under atomic permutations, they are isomorphic to symmetrical superpositions of N spin-1/2 states. These N spin-1/2 states are eigenstates of the angular momentum of a collective-spin system corresponding to the maximum J = N/2 values. This allows to rewrite the collective state as a $|J, M\rangle$ state. Introducing collective operators

$$J^{\pm} = \sum_{i} J_{i}^{\pm} \stackrel{\circ}{=} \sum_{i} D_{i}^{\pm}, \tag{A.4}$$

$$J_3 = \sum_i J_i^3 \stackrel{\circ}{=} \sum_i D_i^3, \tag{A.5}$$

and for completeness

$$J^{2} \stackrel{\circ}{=} D^{2} = \frac{1}{2} \left(D^{+} D^{-} + D^{-} D^{+} \right) + D_{3}^{2}, \tag{A.6}$$

one achieves a similar description as for the known operators of angular momentum in quantum mechanics. Thus, when applying them on a collective state $|J, M\rangle$ one gets

$$J_3 |J, M\rangle = M |J, M\rangle, \qquad (A.7)$$

$$J^{2} |J, M\rangle = J(J+1) |J, M\rangle, \qquad (A.8)$$

$$J^{\pm} |J, M\rangle = \sqrt{J(J+1) - M(M\pm 1)} |J, M\pm 1\rangle.$$
(A.9)

Here, the state $|J, M = 0\rangle$ corresponds to the completely symmetrical state, where J + M atoms are in the excited, and J - M atoms are in the ground state. In this state one observes the maximum emission intensity. When the system reaches $|J, M = -J\rangle$, all atoms are in the ground state and no photons are radiated anymore.

To demonstrate the proportionality of N^2 in the intensity of a superradiant emission, as well as the proportionality of N in the incoherent emission, a short calculation following Haroche and Gross, and Benedict et al. [46,47] is presented.

Consider a system of N two-level atoms, all prepared in their respective excited state. If these atoms act as individual radiators, then the decay will be of exponential form. Let N_{\uparrow} be the number of atoms in the excited state, and τ the mean lifetime. The decay of the excited atoms depends on time and is given by $N_{\uparrow}(t) = Ne^{-t/\tau}$. The intensity of the radiation can then be expressed as

$$I(t) = -\frac{\mathrm{d}N_{\uparrow}(t)}{\mathrm{d}t} = \frac{N}{\tau}e^{-t/\tau}.$$
(A.10)

Thus, the emission intensity is proportional to N, as stated and shown in the upper part of Figure A.1 above.

For the superradiant emission, suppose a system of N coherent radiators is in the maximally excited collective state $|J = N/2, M = +J\rangle$. The emission intensity can be approximated with

$$I(t) = -\frac{\mathrm{d}M(t)}{\mathrm{d}t} = \frac{1}{\tau} \left| \langle M - 1 | J^- | M \rangle \right|^2 = \frac{1}{\tau} \left(J + M(t) \right) \left(J - M(t) + 1 \right).$$
(A.11)

Because of the relation J = N/2, the emission intensity I is proportional to N for $M \approx J$, and proportional to N^2 for $M \approx 0$. For $M(t) \gg 1$, equation (A.11) simplifies to

$$-\frac{\mathrm{d}M(t)}{\mathrm{d}t} = \frac{1}{\tau} \left(J + M(t) \right) \left(J - M(t) \right), \tag{A.12}$$

which can be solved analytically, yielding

$$M(t) = -J \tanh\left(\frac{J}{\tau}(t-t_0)\right) = \frac{N}{2} \tanh\left(\frac{N}{2}\frac{(t-t_0)}{\tau}\right),\tag{A.13}$$

where t_0 is the time when the system is in the fully symmetrical collective state $|J, M = 0\rangle$. Hence, the emission intensity is given by

$$I(t) = \frac{N^2}{4\tau} \frac{1}{\cosh^2\left(\frac{N}{2}\frac{(t-t_0)}{\tau}\right)}.$$
(A.14)

This intensity function has a transient peak around $t \approx t_0$ and reveals the proportionality to N^2 .

B. Quantum Relative Entropy

For this section only, the Boltzmann constant $k_{\rm B}$ is briefly reintroduced to keep apart the entropies of information theory and statistical (quantum) mechanics.

Following classical statistical mechanics, entropy gets introduced through a microcanonical ensemble, where it is assumed that each microscopic state of a macroscopic system is equally probable, if randomly chosen from the ensemble [48,49]. One can then define the Boltzmann entropy of a macroscopic state as

$$S_{\rm B} = k_{\rm B} \log\left(\Omega\right),\tag{B.1}$$

where $k_{\rm B}$ is the Boltzmann constant and Ω is the number of microscopic states, which are consistent with the conditions given by the macroscopic state.

The Boltzmann entropy can be generalized for a system coupled to its surroundings. In general, it does not have to be true that each microscopic state is equally probable, if a system coupled to a heat reservoir is not in thermal equilibrium. Thus for a system with a countable number of microscopic states, one can define the Gibbs entropy as a weighted sum over all microscopic states with probability p_i [50],

$$S_{\rm G} = -k_{\rm B} \sum_{i} p_i \log\left(p_i\right). \tag{B.2}$$

Analogously to the Gibbs entropy, one can define an entropy in information theory. Having some random variable X, the entropy is a measure of the amount of uncertainty, before gaining knowledge about the value of X. Equivalently, it measures the average information gain after learning the value. Given a discrete set of random variables $\{x_i\}$ with probabilities $\{p_i\}$ the entropy is defined as

$$S_{\rm Sh} = -\sum_{i} p_i \log\left(p_i\right),\,$$

which is known as the Shannon entropy [51].

Assume there are two probability distributions $P = \{p_1, ..., p_n\}$ and $Q = \{q_1, ..., q_n\}$, according to [52], one can show the inequality

$$-\sum_{i=1}^{n} p_i \log(p_i) \le -\sum_{i=1}^{n} p_i \log(q_i),$$
 (B.3)

which is known as the Gibbs' inequality [53]. This inequality can be rewritten as

$$\sum_{i=1}^{n} p_i \log\left(\frac{p_i}{q_i}\right) =: D_{\mathrm{KL}}(P||Q) \ge 0, \tag{B.4}$$

which is called the Kullback-Leibler divergence or relative entropy. The equality holds only if both probability distributions are identical. It can be understood as a measure of the difference between two probability distributions [54].

Making a transition to quantum mechanics, the Gibbs entropy discussed above can be extended to a continuous phase space, leading to the von Neumann entropy

$$S_{\rm vN} = -k_{\rm B} {\rm Tr} \left(\rho \log(\rho)\right), \tag{B.5}$$

where ρ is the density matrix of the quantum system. This entropy is widely used in quantum statistical mechanics [e.g. 27, 28, 49–51] and has several important properties [27]. The most important ones for the present work are the two following [35]:

- 1. For all density matrices ρ , it holds that $S_{\rm vN}(\rho) \ge 0$. The equality is true if and only if ρ is a pure state.
- 2. The von Neumann entropy is invariant with respect to unitary transformations U on the same Hilbert space as ρ , i.e. $S_{\rm vN}(U\rho U^{\dagger}) = S_{\rm vN}(\rho)$. Thus, a change of basis of ρ does not change the entropy.

Similarly to the classical relative entropy, a quantum relative entropy can be defined. Let ρ and σ be density matrices. The quantum relative entropy of ρ with respect to σ is given by

$$S(\rho||\sigma) = -k_{\rm B} \text{Tr}\left(\rho \log(\rho)\right) - S_{\rm vN}(\rho) = k_{\rm B} \text{Tr}\left(\rho \left(\log(\rho) - \log(\sigma)\right)\right). \tag{B.6}$$

The quantum relative entropy has several properties [35] but in the present work, there are mainly two of interest.

- 1. It fulfills the inequality $S(\rho || \sigma) \ge 0$ for all ρ and σ . The equality only holds for $\rho = \sigma$.
- 2. The quantum relative entropy is invariant with respect to unitary transformations U, i.e. $S(U\rho U^{\dagger}||U\sigma U^{\dagger}) = S(\rho||\sigma).$

In analogy to the Kullback-Leibler divergence, the quantum relative entropy can be understood as a measure of 'closeness' of two density matrices. Equation (B.6) is useful especially for numerical calculations of thermalizations of systems described by density matrices, if the fully thermalized state is known.

C. Technical Details skipped in Section 4.1

C.1 Going from the Born Approximation to the Markov Approximation

After applying the Born approximation in equation (4.9), the first term on its right-hand side is proportional to $\text{Tr}\left(\hat{B}\hat{\rho}_{\text{B}}\right) =: \langle \hat{B} \rangle$. In Section 2.1, there is a proof given, which shows, that there is always a transformation that sets this quantity to zero. In the same section is also a proof for the time derivative on the left-hand side. Thus, the analogous expression to equation (2.15) is

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -\int_{0}^{t} \mathrm{d}t' \operatorname{Tr}_{\mathrm{B}}\left[\left[\hat{J}_{x}(t) \otimes \hat{B}(t), \left[\hat{J}_{x}(t') \otimes \hat{B}(t'), \hat{\rho}_{\mathrm{S}}(t') \otimes \hat{\rho}_{\mathrm{B}} \right] \right] \right].$$
(C.1)

Following the shown procedure in Section 2.1, equation (C.1) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -\int_{0}^{t} \mathrm{d}t' \left[\hat{J}_{x}(t), \hat{J}_{x}(t')\hat{\rho}_{\mathrm{S}}(t')\right] \mathrm{Tr}\left(\hat{B}(t)\hat{B}(t')\hat{\rho}_{\mathrm{B}}\right) + \left[\hat{\rho}_{\mathrm{S}}(t')\hat{J}_{x}(t'), \hat{J}_{x}(t)\right] \mathrm{Tr}\left(\hat{B}(t')\hat{B}(t)\hat{\rho}_{\mathrm{B}}\right).$$
(C.2)

Defining

$$\operatorname{Tr}\left(\hat{B}(t)\hat{B}(t')\hat{\rho}_{\mathrm{B}}\right) =: \langle \hat{B}(t)\hat{B}(t')\rangle, \qquad (C.3)$$

$$\operatorname{Tr}\left(\hat{B}(t')\hat{B}(t)\hat{\rho}_{\mathrm{B}}\right) =: \langle \hat{B}(t')\hat{B}(t)\rangle, \qquad (C.4)$$

and using the previously proven property $\langle \hat{B}(t)\hat{B}(t')\rangle = \langle \hat{B}(t-t')\hat{B}(0)\rangle$ allows to rewrite the equation to

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -\int_{0}^{t} \mathrm{d}t' \left[\hat{J}_{x}(t), \hat{J}_{x}(t')\hat{\rho}_{\mathrm{S}}(t')\right] \langle \hat{B}(t-t')\hat{B}(0)\rangle + \left[\hat{\rho}_{\mathrm{S}}(t')\hat{J}_{x}(t'), \hat{J}_{x}(t)\right] \langle \hat{B}(-(t-t'))\hat{B}(0)\rangle.$$
(C.5)

Introducing a change of variables by substituting $t - t' =: \tau$ yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -\int_{0}^{t} \mathrm{d}\tau \,\left[\hat{J}_{x}(t), \hat{J}_{x}(t-\tau)\hat{\rho}_{\mathrm{S}}(t-\tau)\right] \langle \hat{B}(\tau)\hat{B}(0)\rangle + \left[\hat{\rho}_{\mathrm{S}}(t-\tau)\hat{J}_{x}(t-\tau), \hat{J}_{x}(t)\right] \langle \hat{B}(-\tau)\hat{B}(0)\rangle.$$
(C.6)

Focusing on the bath-correlation function, it can be expressed as

$$\langle \hat{B}(\tau)\hat{B}(0)\rangle = \operatorname{Tr}\left(\left(\sum_{k}h_{k}b_{k}e^{-i\omega_{k}\tau} + h_{k}^{*}b_{k}^{\dagger}e^{i\omega_{k}\tau}\right)\left(\sum_{q}h_{q}b_{q} + h_{q}^{*}b_{q}^{\dagger}\right)\hat{\rho}_{\mathrm{B}}\right)$$

$$= \sum_{k}\sum_{q}\left[h_{k}h_{q}e^{-i\omega_{k}\tau}\operatorname{Tr}\left(b_{k}b_{q}\hat{\rho}_{\mathrm{B}}\right) + h_{k}h_{q}^{*}e^{-i\omega_{k}\tau}\operatorname{Tr}\left(b_{k}b_{q}^{\dagger}\hat{\rho}_{\mathrm{B}}\right) + h_{k}^{*}h_{q}e^{i\omega_{k}\tau}\operatorname{Tr}\left(b_{k}^{\dagger}b_{q}\hat{\rho}_{\mathrm{B}}\right) + h_{k}h_{q}^{*}e^{i\omega_{k}\tau}\operatorname{Tr}\left(b_{k}^{\dagger}b_{q}\hat{\rho}_{\mathrm{B}}\right) + h_{k}^{\dagger}h_{q}^{\dagger}e^{i\omega_{k}\tau}\operatorname{Tr}\left(b_{k}^{\dagger}b_{q}\hat{\rho}_{\mathrm{B}}\right)\right].$$

$$(C.7)$$

The expectation values appearing in this double sum satisfy the following relations:

$$\operatorname{Tr}\left(b_{k}b_{q}\hat{\rho}_{\mathrm{B}}\right) = \langle b_{k}b_{q}\rangle = 0 \quad \forall \, k, q, \qquad (C.8)$$

$$\operatorname{Tr}\left(b_{k}^{\dagger}b_{q}^{\dagger}\hat{\rho}_{\mathrm{B}}\right) = \langle b_{k}^{\dagger}b_{q}^{\dagger} \rangle = 0 \quad \forall \, k, q,$$
(C.9)

$$\operatorname{Tr}\left(b_{k}^{\dagger}b_{q}\hat{\rho}_{\mathrm{B}}\right) = \langle b_{k}^{\dagger}b_{q} \rangle = 0 \quad \text{for } k \neq q.$$
(C.10)

Applying these properties and the commutation relation $\begin{bmatrix} b_k, b_k^{\dagger} \end{bmatrix} = 1$ leads to

$$\langle \hat{B}(\tau)\hat{B}(0)\rangle = \sum_{k} |h_{k}|^{2} \bigg[e^{-i\omega_{k}\tau} \left(1 + \langle b_{k}^{\dagger}b_{k}\rangle \right) + e^{i\omega_{k}\tau} \langle b_{k}^{\dagger}b_{k}\rangle \bigg].$$
(C.11)

The operators in the expectation values can be identified with number operators. Since they are bosonic, they can be replaced with the Bose-Einstein distribution factor

$$\langle b_k^{\dagger} b_k \rangle = \langle n_k \rangle = n_b(\omega_k) = \left(e^{\omega_k \beta} - 1 \right)^{-1}.$$
 (C.12)

Thus, the bath-correlation function becomes equation (4.11),

$$\langle \hat{B}(\tau)\hat{B}(0)\rangle = \sum_{k} |h_{k}|^{2} \bigg[e^{-i\omega_{k}\tau} \left(1 + n_{b}(\omega_{k})\right) + e^{i\omega_{k}\tau} n_{b}(\omega_{k}) \bigg].$$
(C.13)

Claim: For the bath-correlation function holds $\langle \hat{B}(-\tau)\hat{B}(0)\rangle = \langle \hat{B}(\tau)\hat{B}(0)\rangle^*$.

Proof:

$$\langle \hat{B}(-\tau)\hat{B}(0)\rangle = \sum_{k} |h_{k}|^{2} \left[e^{i\omega_{k}\tau} \left(1 + n_{b}(\omega_{k})\right) + e^{-i\omega_{k}\tau}n_{b}(\omega_{k}) \right]$$
$$= \sum_{k} |h_{k}|^{2} \left[\left(e^{-i\omega_{k}\tau}\right)^{*} \left(1 + n_{b}(\omega_{k})\right) + \left(e^{i\omega_{k}\tau}\right)^{*}n_{b}(\omega_{k}) \right]$$

Since $|h_k|^2$ and $n_b(\omega_k)$ are real, this expression can be reacst, so that

$$= \sum_{k} \left(|h_{k}|^{2} \left[e^{-i\omega_{k}\tau} \left(1 + n_{b}(\omega_{k}) \right) + e^{i\omega_{k}\tau} n_{b}(\omega_{k}) \right] \right)^{*}$$
$$= \left(\sum_{k} |h_{k}|^{2} \left[e^{-i\omega_{k}\tau} \left(1 + n_{b}(\omega_{k}) \right) + e^{i\omega_{k}\tau} n_{b}(\omega_{k}) \right] \right)^{*} = \langle \hat{B}(\tau) \hat{B}(0) \rangle^{*}$$

Returning to equation (C.6), the hermeticity of \hat{J}_x and $\hat{\rho}_S$, as well as the right above proven relation of the bath-correlation function can be used to obtain equation (4.10).

C.2 Going from the Markov Approximation to the Secular Approximation

After obtaining equation (4.24), the spectral decomposition of H_S is used to do an eigenoperator decomposition of $\hat{J}_x(t)$. In complete analogy to Section 2.2, by defining $\omega := \varepsilon_b - \varepsilon_a$, with ε_i being eigenenergies of H_S , the following relations can be found:

$$\hat{J}_x(t) = \sum_{\omega} e^{-i\omega t} J_x(\omega), \qquad (C.14)$$

$$\hat{J}_x^{\dagger}(t) = \sum_{\omega} e^{i\omega t} J_x^{\dagger}(\omega).$$
(C.15)

Note that hereby $J_x(\omega) := \sum_{\varepsilon_b - \varepsilon_a = \omega} \langle \varepsilon_a | J_x | \varepsilon_b \rangle | \varepsilon_a \rangle \langle \varepsilon_b |$ and hence, $J_x(-\omega) = J_x^{\dagger}(\omega)$.

Using equations (C.14) and (C.15), one finds by direct computation

$$[H_{\rm S}, J_x(\omega)] = -\omega J_x(\omega), \qquad (C.16)$$

$$\left[H_{\rm S}, J_x^{\dagger}(\omega)\right] = \omega J_x^{\dagger}(\omega), \qquad (C.17)$$

$$\left[H_{\rm S}, J_x^{\dagger}(\omega) J_x(\omega)\right] = 0. \tag{C.18}$$

Making use of the hermeticity of $\hat{J}_x(t)$, plugging in above decompositions in equation (4.24) and rearranging the terms leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}}(t) = -\sum_{\omega}\sum_{\omega'}\left[\int_{0}^{\infty}\mathrm{d}\tau \left(\langle\hat{B}(\tau)\hat{B}(0)\rangle e^{i\omega'\tau}\right)e^{i(\omega-\omega')t}\left[J_{x}^{\dagger}(\omega), J_{x}(\omega')\hat{\rho}_{\mathrm{S}}(t)\right] + \mathrm{h.c.}\right],\qquad(\mathrm{C.19})$$

which is, after defining $\Gamma(\omega') := \int_{0}^{\infty} d\tau \langle \hat{B}(\tau) \hat{B}(0) \rangle e^{i\omega'\tau}$, equation (4.25).

C.3 Going from the Secular Approximation to the Lindblad Master Equation

In Section 4.1.2 the full Fourier transform of the bath correlation function was given in equation (4.17). This expression for $\gamma(\omega)$ can be written with $\Gamma(\omega)$ due to the linearity of the integral,

$$\begin{split} \gamma(\omega) &= \int_{-\infty}^{\infty} \mathrm{d}\tau \, \langle \hat{B}(\tau) \hat{B}(0) \rangle e^{i\omega\tau} = \int_{-\infty}^{0} \mathrm{d}\tau \, \langle \hat{B}(\tau) \hat{B}(0) \rangle e^{i\omega\tau} + \int_{0}^{\infty} \mathrm{d}\tau \, \langle \hat{B}(\tau) \hat{B}(0) \rangle e^{i\omega\tau} \\ &= \int_{-\infty}^{0} \mathrm{d}\tau \, \langle \hat{B}(\tau) \hat{B}(0) \rangle e^{i\omega\tau} + \Gamma(\omega). \end{split}$$
(C.20)

With the previously proven identity $\langle \hat{B}(-\tau)\hat{B}(0)\rangle = \langle \hat{B}(\tau)\hat{B}(0)\rangle^*$ the first integral after splitting the full Fourier transformation can be expressed as

$$\int_{-\infty}^{0} \mathrm{d}\tau \, \langle \hat{B}(\tau) \hat{B}(0) \rangle e^{i\omega\tau} \stackrel{\tau \to -\nu}{=} \int_{0}^{\infty} \mathrm{d}\nu \, \langle \hat{B}(\nu) \hat{B}(0) \rangle^* e^{-i\omega\nu} = \left(\int_{0}^{\infty} \mathrm{d}\nu \, \langle \hat{B}(\nu) \hat{B}(0) \rangle e^{i\omega\nu} \right)^* = \Gamma^*(\omega). \quad (C.21)$$

Combining equations (C.20) and (C.21) yields

$$\gamma(\omega) = \Gamma^*(\omega) + \Gamma(\omega). \tag{C.22}$$

In order to find equation (4.28), the exact same procedure as in Section 2.3 is carried out. Starting with

$$\Gamma(\omega) = \int_{0}^{\infty} d\tau \, \langle \hat{B}(\tau) \hat{B}(0) \rangle e^{i\omega\tau}, \qquad (C.23)$$

the bath-correlation function gets replaced with its inverse Fourier transform, such that

$$\Gamma(\omega) = \int_{0}^{\infty} \mathrm{d}\tau \, \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega' \, \gamma(\omega') e^{-i\omega'\tau} e^{i\omega\tau}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \gamma(\omega') \int_{0}^{\infty} d\tau \, e^{i(\omega-\omega')\tau}.$$
 (C.24)

Making use of the Sokhotski-Plemelj formula [32], this yields

$$\Gamma(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \gamma(\omega') \left[\pi \delta(\omega - \omega') + i\mathcal{P}\left(\frac{1}{\omega - \omega'}\right) \right]$$
$$= \frac{1}{2}\gamma(\omega) + i\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \gamma(\omega')\mathcal{P}\left(\frac{1}{\omega - \omega'}\right)$$
$$= \frac{1}{2}\gamma(\omega) + i\sigma(\omega).$$
(C.25)

With this and the previously found equation (C.22) one obtains

$$\sigma(\omega) = \frac{1}{2i} \left(\Gamma(\omega) - \Gamma^*(\omega) \right), \qquad (C.26)$$

$$\Gamma^*(\omega) = \frac{1}{2}\gamma(\omega) - i\sigma(\omega).$$
(C.27)

Carrying out the same calculations with equations (C.25) and (C.27) in equation (4.26), one obtains the Lindblad master equation given in equation (4.29).

List of Variables

A_n	operator of a system coupled to an environment
\hat{A}_n	A_n in the interaction picture
$A_n(\omega)$	eigenoperator of $H_{\rm S}$
b_k,b_k^\dagger	bosonic creation and annihilation operator
\hat{B}	short notation for the sum of bosonic operators in \hat{H}_{I}
B_n	environment operator
\hat{B}_n	B_n in the interaction picture
$\bar{B}_{nm}(\tau,0)$	short expression for a bath-correlation function
$\mathcal{D}[\cdot] ho$	Lindblad dissipator
$\langle E_i \rangle$	mean energy at the $i{\rm th}$ position in the quantum Otto cycle, as depicted in Figure 3.1
g	coupling strength parameter
h_k	mode strength of the bosonic bath oscillators
\mathscr{H}	Hilbert space to $H(t)$
\mathscr{H}_{B}	Hilbert space to $H_{\rm B}$
\mathcal{H}_{S}	Hilbert space to $H_{\rm S}$
H(t)	Hamiltonian of an open quantum system
$\hat{H}(t)$	Hamiltonian of an open quantum system in the interaction picture
$H_{\rm B}$	Hamiltonian of an environment/heat bath
H_{I}	Hamiltonian describing the interaction between $H_{\rm S}$ and $H_{\rm B}$
$H_{ m LS}$	Lamb shift Hamiltonian
$H_{\rm S}$	Hamiltonian of a working fluid
H_0	free part of the Hamiltonian $H(t)$
J_z	collective-spin operator
$J_x(\omega)$	eigenoperator of $H_{\rm S}$
J_{\pm}	collective-ladder operators
J_0	strength of the collective coupling to the heat bath
$J(\omega)$	spectral density function
$L_{a,b}$	Lindblad operators in a basis that diagonalizes $H_{\rm S}$
$n_b(\omega)$	Bose-Einstein distribution factor
N	number of two-level systems in the working fluid, $N = 2j$
$S(ho_i ho_{ m th})$	quantum relative entropy of ρ_i with respect to $\rho_{\rm th}$
$S_{nm}(\omega)$	expression of an integral involving $\gamma_{nm}(\omega)$ and a Cauchy principal value
$t_{ m th}$	thermalization time
T_c	temperature of the cold heat bath
T_h	temperature of the hot heat bath
Р	power output
Q_c	heat transferred from the working fluid to a heat bath

Q_h	heat transferred from a heat bath to a working fluid
W	extracted work per cycle in the quantum Otto heat machine
α^{\pm}	Clebsch-Gordan coefficients in the rate equations
β	inverse temperature
γ	constant dissipation rate in the non-interacting collective-spin model
$\gamma_{nm}(\omega)$	Fourier transformation of the bath-correlation function
$\gamma(\omega)$	Fourier transformation of the bath-correlation function in the quadratic model
$\Gamma(\omega)$	half-range Fourier transformation of the bath-correlation function in the quadratic model
$\Gamma_{nm}(\omega)$	half-range Fourier transformation of the bath-correlation function
ε	tolerance value to determine the bath-correlation time $\tau_{\rm B}$
ε_i	eigenvalue of $H_{\rm S}$
η	efficiency of a quantum Otto cycle
η_C	Carnot efficiency
λ	dimensionless control parameter
λ_f	control parameter during the thermal stroke 2 \longrightarrow 3, as depicted in Figure 3.1
λ_i	control parameter during the thermal stroke 4 \longrightarrow 1, as depicted in Figure 3.1
$ ho_i$	initial state
$ ho_{ m th}$	fully thermalized Gibbs state
ho(t)	density matrix of the composite quantum system
$\hat{ ho}(t)$	density matrix of the composite quantum system in the interaction picture
$\hat{ ho}_{ m B}$	time-independent, stationary bath state
$ ho_{ m S}(t)$	density matrix of the system
$\hat{ ho}_{ m S}(t)$	density matrix of the system in the interaction picture
$\sigma(\omega)$	expression of an integral involving $\gamma(\omega)$ and a Cauchy principal value
$ au_{ m B}$	time scale for which the bath-correlation function decays to zero
$ au_{ m R}$	relaxation time of the system; thermalization time
$ au_{ m S}$	time scale for the evolution of the working fluid
ω	difference of two eigenvalues of $H_{\rm S}$
ω_c	cut-off frequency
ω_k	frequency of the bosonic bath
ω_0	energy scaling factor

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