Dissipative dynamics of a biased qubit coupled to a harmonic oscillator: analytical results beyond the rotating wave approximation

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Abstract. We study the dissipative dynamics of a biased two-level system (TLS) coupled to a harmonic oscillator (HO), the latter interacting with an Ohmic environment. Using the Van Vleck perturbation theory and going to second order in the coupling between the TLS and the HO, we show how the Hamiltonian of the TLS–HO system can be diagonalized analytically. Our model represents an improvement on the usually used Jaynes–Cummings Hamiltonian as an initial rotating wave approximation is avoided. By assuming a weak coupling to the thermal bath, analytical expressions for the time evolution of the populations of the TLS are found: the population is characterized by a multiplicity of damped oscillations together with a complex relaxation dynamics towards thermal equilibrium. The long time evolution is characterized by a single relaxation rate, which is largest at resonance and whose expression can be given in a closed analytic form.

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1. Introduction

In recent years, the spin-boson model [1–3] has experienced a strong revival, as it is well suited to describe dissipative and decoherence effects on the dynamics of a two-level system (TLS) or qubit coupled to a bath. Crucial for the effects of the environment on the dynamics of the TLS is the shape of the spectral density of the harmonic bath. It is common to assume an Ohmic spectral density, which is linear in the continuous bath modes. In this work, we concentrate on a so-called structured bath, for which the spectral density is Ohmic at low frequencies but exhibits a Lorentzian-shaped peak at a certain frequency $\Omega_1$. It has been shown in [4] that a spin-boson model with such an effective spectral density can be exactly mapped on the model of a TLS which is coupled to a single harmonic oscillator (HO) of frequency $\Omega$, where the latter feels the influence of an Ohmic bath.
Due to its wide applicability the TLS–oscillator system has been the subject of intense research over the years. So, it reflects for example the physics of single atoms with a large electric dipole moment coupled to the microwave photons of a cavity [5], or quantum dots in photonic crystals [6, 7]. More recently the model has received quite a bit of attention in the field of quantum computation, where TLSs are used to implement the two logical states of a qubit. We will especially focus on the solid-state implementation of such systems. Here, two prominent realizations of a qubit–oscillator system are the Cooper-pair box (CPB) [8]–[11] coupled to a transmission line resonator [12]–[17] and the Josephson flux qubit [18] read out by a dc-SQUID [19]–[22]. Inspired by experiments with real atoms interacting with a cavity mode, one speaks for the CPB case of circuit quantum electrodynamics, as now the CPB plays the role of an artificial atom and the waveguide acts as a cavity. From such a setup one expects a huge step towards the realization of a quantum computer, as the transmission line resonator can be used to couple qubits together [9, 23], store the information of qubits or to provide non-demolition read-out schemes [12, 15]. Concerning the flux qubit, the read-out usually happens through a damped dc-SQUID, which is inductively coupled to the qubit. However, through the SQUID environmental noise is transferred to the qubit leading to decoherence and dissipation within its dynamics. The effect of this noise on the qubit depends very much on the strength $g$ of the coupling between qubit and SQUID and one faces a conflicting situation. On the one hand one wants a strong coupling for a good read-out resolution. On the other hand the coupling should be minimized to keep the negative effects of the environment as small as possible. In [24, 25], it has been shown that the qubit-SQUID system can be described by a spin-boson model with an effective spectral density $G_{\text{eff}}(\omega)$ exhibiting a peak at the plasma frequency $\Omega_1$ of the SQUID. Applying the above mentioned mapping an equivalent point of view is to consider the SQUID as an LC-circuit coupled to the Ohmic bath and model it as a HO. A detailed description of a non-destructive read-out scheme is e.g. given in [26].

The spin-boson model can be formally solved using e.g. real-time path integral methods [1, 2]. However, in order to get closed-form analytical results, approximations must be invoked. A quite common one is the so-called weak coupling approximation (WCA), which is perturbative in the bath spectral density [2]. However, it has been shown that for strong qubit–HO coupling $g$ and for small detuning $\delta = \Omega - \Delta_b$, where $\Delta_b$ is the qubit energy splitting, such an approximation breaks down [27], as coherent exchange processes between the TLS and the oscillator are disregarded. For an unbiased qubit, the non-interacting blip approximation (NIBA) used in [28]–[31] circumvents this problem as it is non-perturbative in the coupling $g$ and therefore takes correctly into account the influence of the oscillator on the TLS. Moreover, it allows an analytic treatment of the dynamics. However, the NIBA is known to break down for a biased qubit at low temperatures [1, 2]. Another approach, which treats the system non-perturbatively in the bath, is the flow-equation renormalization method [32, 33], where the spin-boson Hamiltonian is diagonalized using infinitesimal unitary transformations. However, within this approach analytical solutions are difficult to find. Recently a polaron transformation was used by Huang et al to obtain analytically the population dynamics and confirm Shiba’s relation for an unbiased TLS [34].

In the case in which the qubit and the HO are considered as the central quantum system being coupled to an Ohmic bath, the numerical, \textit{ab initio} quasi-adiabatic propagator path-integral (QUAPI) method [35, 36] is a nice tool as it enables one to cover both the resonant regime, where the oscillator frequency is close to the qubit energy splitting, and the dispersive regime with the oscillator being far detuned from the qubit [27, 29, 30]. Moreover, it can be
applied to a biased as well as to an unbiased TLS and therefore can be used as a testbed for analytical results. For qubits being operated at the degeneracy point, which means an unbiased TLS, very often a rotating wave approximation (RWA) is applied [12], which is expected to be valid for small detuning and yields as starting point the Jaynes–Cummings Hamiltonian [37, 38]. This model was first used to study a two-state atom interacting with a single, close to resonance cavity mode of the electromagnetic field and predicts e.g. the repeated revival and collapse of Rabi oscillations within the atomic excitation probability. By considering the TLS–HO system in the representation of displaced HO states, Brito et al were able to truncate the infinite Hilbert space of this system without losing the effects of the HO on the TLS dynamics [39]. However, so far none of these works could provide an analytical expression for the dynamics of the dissipative qubit being valid for zero as well as nonzero detuning and for both a biased and unbiased TLS. In this work, an analytic expression for the dissipative qubit’s dynamics which includes the effects of a finite detuning and of a static bias is derived. Specifically, starting from the qubit–HO perspective, the eigenvalues and eigenfunctions of the non-dissipative TLS–HO system are found approximately using the Van Vleck perturbation theory up to second order in the coupling $g$. Notice that no RWA is required. Dissipation effects are then evaluated by solving a Born–Markov master equation for the reduced density matrix in the system’s eigenbasis.

The structure of the work is as follows. The dissipative TLS–HO Hamiltonian and the main dynamical quantities are introduced in section 2. Inspired by the work of Goorden et al [29, 30], we demonstrate in section 3 how the eigenstates and eigenenergies of the non-dissipative Hamiltonian can be found approximately using the Van Vleck perturbation theory [40, 41]. In this way, we can provide an analytical formula for the non-dissipative dynamics which takes into account the full Hilbert space of the qubit–HO system. After that, we show how for low temperatures ($k_B T < \hbar \Omega, \hbar \Delta_b$) this infinite Hilbert space can be truncated and discuss the relevant contributions of the HO to the dynamics. In section 4, the influence of the environment is investigated, by looking at solutions of the Bloch–Redfield equations. Specifically, analytical expressions for the TLS dynamics are obtained and compared with numerical solutions. The main physical features of the coupled TLS–HO system are discussed in section 5. To illustrate the effects of counter-rotating terms in the Hamiltonian of the qubit–HO system, which are neglected when performing a RWA, we compare in section 6 our calculations to results obtained from the Jaynes–Cummings model.

2. The model

In this section, we introduce the Hamiltonian for a qubit coupled through a HO to a thermal bath. Further, a formula for the population difference between the qubit’s two logical states is derived.

2.1. The qubit–oscillator–bath system

To setup the model, we consider the Hamiltonian of a qubit–HO system, $\mathcal{H}_{QHO}$, which is coupled to an environmental bath, $\mathcal{H}_B$, by the interaction Hamiltonian $\mathcal{H}_{OB}$, so that the total Hamiltonian becomes

$$\mathcal{H} = \mathcal{H}_{QHO} + \mathcal{H}_{OB} + \mathcal{H}_B.$$
The Hamiltonian, $\mathcal{H}_{\text{QHO}} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}$, consists of

$$\mathcal{H}_0 = \mathcal{H}_{\text{TLS}} + \mathcal{H}_{\text{HO}} = -\frac{\hbar}{2}(\varepsilon \sigma_z + \Delta_0 \sigma_z) + \hbar \Omega B^\dagger B,$$

the Hamiltonian of the TLS/qubit and the HO, and the interaction term

$$\mathcal{H}_{\text{int}} = \hbar g \sigma_z (B^\dagger + B).$$

(3)

The Hamiltonian of the TLS is given in the subspace $\{ |L\rangle, |R\rangle \}$, corresponding to a clockwise or counterclockwise current in the superconducting loop of a three-junction Josephson qubit or more generally to the qubit’s two logical states. In the case of a superconducting flux-qubit, the energy bias $\varepsilon$ can be tuned by an applied external flux, $\Phi_{\text{ext}}$, and is zero at the so-called degeneracy point. The tunnelling amplitude is described by $\Delta_0$. For $\varepsilon \gg \Delta_0$, the states $|L\rangle$ and $|R\rangle$ are eigenstates of $\mathcal{H}_{\text{TLS}}$, whereas at the degeneracy point those eigenstates are a symmetric and antisymmetric superposition of the two logical states. Further, $B$ and $B^\dagger$ are the annihilation and creation operator for the HO with frequency $\Omega$, and $g$ characterizes the coupling strength.

We also introduce the energy splitting $\hbar \Delta_b \equiv \hbar \sqrt{\varepsilon^2 + \Delta_0^2}$ between the ground state $|g\rangle$ and the excited state $|e\rangle$ of the TLS. Using the transformation

$$R(\Theta) = \begin{pmatrix} \cos(\Theta/2) & \sin(\Theta/2) \\ -\sin(\Theta/2) & \cos(\Theta/2) \end{pmatrix}$$

(4)

with $\tan \Theta = -\Delta_0/\varepsilon$ and $-\frac{\pi}{2} \leq \Theta < \frac{\pi}{2}$, we obtain the Hamiltonian of the TLS in the basis:

$$\tilde{\mathcal{H}}_{\text{TLS}} = R^T(\Theta) \mathcal{H}_{\text{TLS}} R(\Theta) = -\frac{\hbar \Delta_b}{2} \tilde{\sigma}_z.$$ 

The states $|R\rangle$ and $|L\rangle$ become in the energy basis

$$|R\rangle = \cos(\Theta/2)|g\rangle + \sin(\Theta/2)|e\rangle,$$

(5)

$$|L\rangle = -\sin(\Theta/2)|g\rangle + \cos(\Theta/2)|e\rangle.$$

(6)

The Hamiltonian $\mathcal{H}_{\text{HO}}$ is diagonal in the eigenbasis $\{|j\rangle\}$ with $j = 0, \ldots, \infty$ being the occupation number: $\mathcal{H}_{\text{HO}} = \sum_j \hbar j \Omega |j\rangle \langle j|$. For the eigenbasis of the combined Hamiltonian $\tilde{\mathcal{H}}_0 \equiv \tilde{\mathcal{H}}_{\text{TLS}} + \mathcal{H}_{\text{HO}}$, we write

$$\{|j\rangle \otimes |g\rangle; |j\rangle \otimes |e\rangle \} \equiv \{|jg\rangle; |je\rangle\}.$$  

(7)

Following Caldeira and Leggett [42], we model the environmental influences originating from the circuitry surrounding the qubit and the oscillator as a bath of HOs being coupled bilinearly to the HO. Thus, the environment is described by $\mathcal{H}_B = \sum_k \hbar \omega_k b_k^\dagger b_k$ and the interaction Hamiltonian is

$$\mathcal{H}_{\text{OB}} = (B^\dagger + B) \sum_k \hbar v_k b_k^\dagger b_k + (B^\dagger + B)^2 \sum_k \hbar \frac{v_k^2}{\omega_k}.$$  

(8)

The operators $b_k^\dagger$ and $b_k$ are the creation and destruction operators, respectively, for the $k$th bath oscillator, $\omega_k$ is its frequency and $v_k$ gives the coupling strength. The whole bath can be described by its spectral density, which we consider to be Ohmic:

$$G_{\text{Ohm}}(\omega) = \sum_k v_k^2 \delta(\omega - \omega_k) = \kappa \omega.$$  

(9)
In [4], it is shown that the above model is equivalent to that of a TLS being coupled directly to a harmonic bath including the single oscillator of frequency \( \Omega \); i.e. a spin-boson model [1, 2] with a peaked effective spectral density,

\[
G_{\text{eff}} = \frac{2\alpha \omega \Omega^4}{(\Omega^2 - \omega^2)^2 + (2\pi \kappa \omega \Omega)^2}.
\]

(10)

The relation between \( \alpha \) and the coupling parameter \( g \) between the qubit and the HO is \( g = \sqrt{\alpha/(8\kappa)} \) [24, 25]. This second perspective is suitable for calculating the dynamics of the qubit using a path-integral approach, as it was done for example in [31] for the case of an unbiased qubit (\( \epsilon = 0 \)). The approach in [31], however, being based on the NIBA [2], is not suitable to investigate the low temperature dynamics of a biased TLS. Thus, in this paper we will consider the TLS and the single oscillator as central quantum system and solve the Bloch–Redfield master equations for the density matrix of this system, which are valid also for the case of a biased TLS.

2.2. The population difference

The main goal of this work is to determine the dynamics \( P(t) \) of the qubit. That means, we wish to calculate the population difference

\[
P(t) = \text{Tr}_{\text{TLS}}\{\sigma_z \rho_{\text{red}}(t)\} = \langle R | \rho_{\text{red}}(t) | R \rangle - \langle L | \rho_{\text{red}}(t) | L \rangle
\]

(11)

between the \( |R\rangle \) and \( |L\rangle \) states of the qubit. The reduced density matrix of the TLS,

\[
\rho_{\text{red}}(t) = \text{Tr}_{\text{HO}}\{\rho(t)\} = \text{Tr}_{\text{HO}}\text{Tr}_{\text{B}}\{W(t)\}
\]

(12)

is found after tracing out the oscillator and bath degrees of freedom from the total density matrix \( W(t) = e^{-\frac{i}{\hbar}Ht} W(0) e^{\frac{i}{\hbar}Ht} \). In turn \( \rho(t) = \text{Tr}_{\text{B}}\{W(t)\} \) is the reduced density matrix of the qubit–HO system. How to calculate this density matrix will be shown later. After some algebra, illustrated in more detail in appendix A, we arrive at an expression for \( P(t) \), given in terms of diagonal and off-diagonal elements of \( \rho(t) \) in the TLS–HO eigenbasis \( \{|n\rangle\} \). It reads

\[
P(t) = \sum_n p_{nn}(t) + \sum_{n \neq m} p_{nm}(t)
\]

(13)

where

\[
p_{nn}(t) = \sum_j \left\{ \cos \Theta \left[ \langle jg|n \rangle^2 - \langle je|n \rangle^2 \right] + 2 \sin \Theta \langle jg|n \rangle \langle je|n \rangle \right\} \rho_{nn}(t),
\]

(14a)

\[
p_{nm}(t) = 2 \sum_j \left\{ \cos \Theta \left[ \langle jg|n \rangle \langle m|jg \rangle - \langle je|n \rangle \langle m|je \rangle \right] + \sin \Theta \left[ \langle je|n \rangle \langle m|jg \rangle + \langle je|m \rangle \langle n|jg \rangle \right] \right\} \text{Re}\{\rho_{nm}(t)\}
\]

(14b)

with \( \rho_{nm}(t) = \langle n|\rho(t)|m \rangle \). How to determine the eigenstates of \( \mathcal{H}_{\text{QHO}} \) is described in the next section.
Figure 1. Energy spectrum of the coupled TLS–HO system versus the oscillator frequency \( \Omega \). Solid lines show the energy levels for the five lowest energy states with the coupling being switched on \((g = 0.18)\) and the TLS being unbiased \((\varepsilon = 0)\). Frequencies and energies are given in units of \( \Delta_0 \) and \( \hbar \Delta_0 \), respectively. For comparison the energy levels for the uncoupled case are also given (dashed lines). At resonance \((\Omega = \Delta_b)\) the spectrum exhibits avoided crossings, whereas it approaches the uncoupled case away from resonance. The vertical dashed lines visualize three different situations: the negatively detuned regime (line a), the resonant case (line b) and the positively detuned regime (line c).

3. Energy spectrum and dynamics of the non-dissipative TLS–HO system

In this section, we show how to find the eigenvalues of the unperturbed qubit–HO Hamiltonian \( \mathcal{H}_{QHO} \) approximately by using the Van Vleck perturbation theory [40, 41]. The idea is to take advantage of the degenerate or doublet structure of the energy spectrum of the uncoupled \((g = 0)\) TLS–HO system near resonance, e.g. at \( \Delta_b \approx \Omega \). Then, as long as the perturbation is small compared with the energy separation of the different doublets, the full Hamiltonian will exhibit a similar spectrum of bundled energy levels.

3.1. Energy spectrum

The eigenenergies of the uncoupled TLS–HO system are immediately found by applying the Hamiltonian \( \tilde{\mathcal{H}}_0 = \tilde{\mathcal{H}}_{TLS} + \mathcal{H}_{HO} \) on the eigenstates in (7):

\[
\tilde{\mathcal{H}}_0 |jg\rangle = \left( -\frac{\hbar \Delta_b}{2} + \hbar j \Omega \right) |jg\rangle \quad \text{and} \quad \tilde{\mathcal{H}}_0 |je\rangle = \left( \frac{\hbar \Delta_b}{2} + \hbar j \Omega \right) |je\rangle.
\]  

(15)

The dashed lines in figure 1 show the energy spectrum corresponding to (15) versus the oscillator frequency \( \Omega \) for the five lowest eigenstates. Except for the ground state, \(|0g\rangle\), the
states \((j+1)g\) and \(je\) are degenerate in the resonant case \((\Omega = \Delta_b)\). Close to resonance the spectrum exhibits a doublet structure. With the coupling being switched on, the full Hamiltonian \(\mathcal{H}_{\text{QHO}}\) reads
\[
\tilde{\mathcal{H}}_{\text{QHO}} \equiv R^\dagger \mathcal{H}_{\text{QHO}} R = \tilde{\mathcal{H}}_0 + \tilde{\mathcal{H}}_{\text{Int}} = \frac{\hbar}{2} \tilde{\sigma}_z + \hbar \Omega B^\dagger B + \hbar g \left( \frac{\varepsilon}{\Delta_b} - \frac{\Delta_0}{\Delta_b} \right) (B + B^\dagger)
\]
(16)
in the basis \(\{|jg\}; |je\}\). In order to diagonalize the Hamiltonian \(\tilde{\mathcal{H}}_{\text{QHO}}\), we consider \(\tilde{\mathcal{H}}_{\text{Int}}\) as a small perturbation, which is reasonable as long as \(g \ll \Delta_b, \Omega\). Applying the Van Vleck perturbation theory, we construct an effective Hamiltonian,
\[
\tilde{\mathcal{H}}_{\text{eff}} = e^{iS} \tilde{\mathcal{H}}_{\text{QHO}} e^{-iS},
\]
(17)
having the same eigenvalues as \(\tilde{\mathcal{H}}_{\text{QHO}}\) but no matrix elements connecting states which are far off from degeneracy. Thus, \(\tilde{\mathcal{H}}_{\text{eff}}\) will be block-diagonal with all quasi-degenerate energy levels being in one common block. As in our case always two states are nearly degenerate, each block of \(\tilde{\mathcal{H}}_{\text{eff}}\) builds a two-by-two matrix. This can be easily diagonalized in order to determine the eigenstates. Following [40, 41], we calculate the transformation matrix \(S\) up to second order in \(g\). The general formulae for both an arbitrary Hamiltonian and \(\tilde{\mathcal{H}}_{\text{QHO}}\) are given in appendix B. The only surviving matrix elements of the effective Hamiltonian, apart from the ones being of zeroth order in \(g\), are
\[
\begin{align*}
\left(\tilde{\mathcal{H}}_{\text{eff}}\right)_{j,e;(j+1)g}^{(1)} & = \hbar \Delta \sqrt{j+1} \quad \text{with} \quad \Delta = -\frac{g \Delta_0}{\Delta_b}, \\
\left(\tilde{\mathcal{H}}_{\text{eff}}\right)_{j,e;j,e}^{(2)} & = -\frac{\hbar \varepsilon^2}{\Delta_b^2 \Omega} g^2 + j \frac{\hbar \Delta_0^2}{\Delta_b^2 (\Delta_b + \Omega)} g^2 \equiv \hbar (W_1 - j W_0),
\end{align*}
\]
(18)
and
\[
\left(\tilde{\mathcal{H}}_{\text{eff}}\right)_{j,g;j,g}^{(2)} = \hbar [W_1 + (j+1) W_0].
\]
(19)
Thus, \(\tilde{\mathcal{H}}_{\text{eff}} = \tilde{\mathcal{H}}_{\text{eff}}^{(0)} + \tilde{\mathcal{H}}_{\text{eff}}^{(1)} + \tilde{\mathcal{H}}_{\text{eff}}^{(2)}\) has the matrix structure
\[
\begin{pmatrix}
\ddots & \ddots & \ddots \\
\Delta_0 + j \Omega + W_1 - j W_0 & \sqrt{j+1} \Delta \\
\sqrt{j+1} \Delta & -\Delta_0 + (j+1) \Omega + W_1 + (j+2) W_0 \\
\ddots & \ddots & \ddots
\end{pmatrix},
\]
(21)
where the section shown corresponds to the basis states \(|je\) and \(|(j+1)g\). From this form it is easy to calculate the eigenstates and eigenenergies. The ground state \(|0\rangle_{\text{eff}} \equiv |0g\rangle\), which is an eigenstate of \(\tilde{\mathcal{H}}_{\text{eff}}\), has the eigenenergy
\[
E_0 = \hbar \left(-\frac{\Delta_b}{2} + W_0 + W_1\right).
\]
(22)
The other eigenstates of $\tilde{H}_{\text{eff}}$ are, $j \geq 0$,

$$|2j+1\rangle_{\text{eff}} = \cos\left(\frac{\alpha_j}{2}\right) |(j+1)g\rangle + \sin\left(\frac{\alpha_j}{2}\right) |je\rangle,$$

$$|2j+2\rangle_{\text{eff}} = -\sin\left(\frac{\alpha_j}{2}\right) |(j+1)g\rangle + \cos\left(\frac{\alpha_j}{2}\right) |je\rangle,$$

(23a, 23b)

corresponding to the eigenenergies

$$E_{2j+1/2j+2} = \hbar \left[ \left( j + \frac{1}{2} \right) \Omega + W_1 + W_0 \mp \frac{\delta_j}{2 \cos\alpha_j} \right],$$

$$= \hbar \left[ \left( j + \frac{1}{2} \right) \Omega + W_1 + W_0 \mp \frac{1}{2} \sqrt{\delta_j^2 + 4(j+1)|\Delta|^2} \right],$$

(24)

with

$$\delta_j = \Delta_b - \Omega - 2(j+1)W_0, \quad \tan\alpha_j = \frac{2\sqrt{j+1}|\Delta|}{\delta_j} \quad \text{and} \quad 0 \leq \alpha_j < \pi.$$  

(25)

By construction, these are also eigenenergies of $\tilde{H}_{\text{QHO}}$. Using the transformation (17), we get the eigenvectors of $\tilde{H}_{\text{QHO}}$ as

$$|0\rangle = e^{-is}|0\rangle_{\text{eff}}, \quad |2j+1\rangle = e^{-is}|2j+1\rangle_{\text{eff}} \quad \text{and} \quad |2j+2\rangle = e^{-is}|2j+2\rangle_{\text{eff}}.$$  

(26)

The energy spectrum of $\tilde{H}_{\text{QHO}}$ is shown in figure 1 for the case of an unbiased TLS ($\varepsilon = 0$). We want to emphasize that our findings are also valid for the more general case $\varepsilon \neq 0$. At resonance, where the spectrum for the uncoupled case is degenerated, avoided crossings can be seen. The gap between two formerly degenerated levels for $\Omega = \Delta_b$ is

$$E_{2j+2} - E_{2j+1} = 2\hbar \sqrt{j+1}g + O(g^3),$$

(27)

which is as predicted by the Jaynes–Cumming model [37, 38]. As we will show in section 6, the second-order correction $W_0$ in (21), which leads to a shift in the resonance frequency, is a result of the counter-rotating terms in $\tilde{H}_{\text{QHO}}$. As such it can be interpreted as a Bloch–Siegert shift [43].

3.2. Dynamics of the qubit for the non-dissipative case

With the coupling to the bath being turned off, the time evolution of the density matrix of the qubit–HO system is given by $\rho(t) = e^{-i/\hbar \tilde{H}_{\text{QHO}}} \rho(0) e^{i/\hbar \tilde{H}_{\text{QHO}}} \rho(t)$ and consequently

$$\rho_{nm}(t) = \langle n|\rho(t)|m \rangle = e^{-i\omega_{nm}t} \rho_{nm}(0)$$

(28)

with $\omega_{nm} = \frac{1}{\hbar}(E_n - E_m)$. With that (13) becomes

$$P(t) = p_0 + \sum_{n > m} p_{nm}(0) \cos \omega_{nm} t,$$

(29)

where we defined $p_0 = \sum_n p_{nn}(0)$. From (29), we notice that the dynamics of the qubit is characterized by an infinite number of oscillation frequencies rather than showing Rabi oscillations with a single distinct frequency. This is clearly a consequence of the coupling of
the HO to the TLS. Further we assume that at \( t = 0 \) the qubit starts in the state \( |R\rangle \) and that the occupation numbers of the HO are Boltzmann distributed, so that

\[
\rho(0) = |R\rangle\langle R| \frac{1}{Z} e^{-\beta \hat{H}_{\text{HO}}},
\]

where \( Z = e^{\beta \Omega / 2} / (1 - e^{-\beta \Omega}) \) is the partition function of the oscillator and \( \beta = (k_B T)^{-1} \) denotes the inverse temperature of the system. In the TLS–HO eigenbasis, this becomes

\[
\rho_{nn}(0) = \langle n|\rho(0)|n\rangle = \frac{1}{Z} \sum_{j=0}^{\infty} e^{-\beta \Omega (j+1/2)} \left[ \cos \left( \frac{\Theta}{2} \right) \langle n|j\rangle + \sin \left( \frac{\Theta}{2} \right) \langle n|j\epsilon\rangle \right] 
\times \left[ \cos \left( \frac{\Theta}{2} \right) \langle j\epsilon|m\rangle + \sin \left( \frac{\Theta}{2} \right) \langle j\epsilon|m\rangle \right].
\]

### 3.3. Low temperature approximation

With (29) we found a formula which describes using the approximate eigenenergies and eigenstates in (24) and (26) the non-dissipative dynamics up to second order in \( g \), thereby taking into account all oscillator levels. Thus, we still have to deal with an infinite Hilbert space. Typically experiments, see e.g. in [13, 21], run in a temperature regime for which \( \beta^{-1} \lesssim \hbar \Omega, \hbar \Delta_b \). Considering the exponential function in (31) we assume the higher oscillator levels to be only sparsely populated and the maximum value of the sum in (31) is truncated to \( j = 1 \). Nevertheless, states \( |j\epsilon\rangle \) with \( j > 1 \) still play a role in the dynamics. In fact, due to the Van Vleck transformation \( \exp(-iS) \), for example the state

\[
|8\rangle = e^{-iS}|8\rangle_{\text{eff}} = e^{-iS} \left[ -\sin \left( \frac{\alpha_3}{2} \right) |4\rangle + \cos \left( \frac{\alpha_3}{2} \right) |3\epsilon\rangle \right]
\]

yields non-vanishing contributions to the matrix elements \( \langle n|1\rangle \) and \( \langle n|1\epsilon\rangle \) occurring in (31) due to the fact that the energy eigenstates (26) of the coupled TLS–HO system are made of linear combinations which also involve these states.

Using (146) together with (28) one finds that coefficients \( p_{nm}(0) \) with \( n \geq 7 \) are of higher than second order in \( g \). The same is valid for \( p_{50}, p_{60}, p_{55} \) and \( p_{66} \). Thus, those terms play no role in our calculation of \( P(t) \). Furthermore, \( e^{-(3/2)\beta \Omega} (g/\Delta_b \Omega)^2 \ll 1 \). Neglecting also these contributions we find that \( p_{n,m} \ll 1 \) for \( n \geq 5 \). In the end it will be sufficient to concentrate on eigenstates of \( \hat{H}_{\text{QHO}} \) up to \( |4\rangle \). This truncation leaves us with ten possible oscillation frequencies \( \omega_{nm} \), where \( n, m = 0, 1, \ldots, 4 \) and \( n > m \).

As an example, we calculate the dynamics of an unbiased TLS (\( \epsilon = 0 \)). Here the coefficients \( p_0, p_{30}(0), p_{40}(0), p_{21}(0) \) and \( p_{43}(0) \) vanish due to symmetry, so that

\[
P(t) = p_{10} \cos (\omega_{10} t) + p_{20} \cos (\omega_{20} t) + p_{31} \cos (\omega_{31} t) + p_{41} \cos (\omega_{41} t) 
+ p_{32} \cos (\omega_{32} t) + p_{42} \cos (\omega_{42} t).
\]

Additionally as a benchmark we consider the mostly studied resonant case, where \( \Omega = \Delta_b = \Delta_0 \). In this case we find with (24) the transitions frequencies

\[
\omega_{10} = \Delta_0 - g, \quad \omega_{20} = \Delta_0 + g, \quad \omega_{31} = \Delta_0 + (1 - \sqrt{2})g, \quad \omega_{41} = \Delta_0 + (1 + \sqrt{2})g, \quad \omega_{32} = \Delta_0 - (1 + \sqrt{2})g, \quad \omega_{42} = \Delta_0 - (1 - \sqrt{2})g.
\]

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The dynamical quantity $P(t)$ and its Fourier transform are shown in figure 2. One clearly sees the influence of the coupling to the HO on the dynamics of the TLS. Instead of Rabi oscillations with a single frequency, $P(t)$ oscillates with six different frequencies, which are in the Fourier spectrum symmetrically located around the point $\omega = \Delta_0$. Among those frequencies $\omega_{10}$ and $\omega_{20}$ are dominating. They correspond to transitions between the first or second energy level of the qubit–HO system and its ground state and their weight is almost equal. To summarize, one notices that due to the coupling with the oscillator additional frequencies are induced into the qubit dynamics. Theoretically, the number of those frequencies is infinite. At low temperatures, however, transitions between the lower energy levels of the system are clearly dominating. Again, for simplicity we have shown here the case of an unbiased TLS. For $\epsilon \neq 0$, the behaviour is similar only that in the Fourier spectrum the weight difference of the two dominating peaks will be more pronounced.

4. The influence of the environment

In the preceding section, we neglected the influence of the bath on the qubit–HO system. Yet, in order to model a realistic situation, we have to pay attention to environmental influences, as they lead to decoherence and dissipation in the dynamics of the qubit, which is harmful for quantum computing application. Thus, we will now consider the full Hamiltonian $\mathcal{H}$.

4.1. Master equation for the qubit–HO system

As shown in section 2.2, we need for the calculation of the population difference $P(t)$ the density matrix $\rho(t)$ of the qubit–HO system. Starting from the Liouville equation of motion for
the full density matrix $W(t)$ of $\mathcal{H}$,

$$i\hbar \frac{\partial W(t)}{\partial t} = [\mathcal{H}_{\text{QHO}}(t)_1, W(t)_1].$$

where the index stands for the interaction picture and following [44, 45], we can provide a Born–Markov master equation for $\rho(t)$ being in the Schrödinger picture and expressed in the basis of the eigenstates of $\tilde{\mathcal{H}}_{\text{QHO}}$:

$$\dot{\rho}_{nm}(t) = -i\omega_{nm}\rho_{nm}(t) + \pi \sum_{kl} \mathcal{L}_{nm,kl}\rho_{k,l}(t).$$

The free dynamics of the system is given by the first term of the right-hand side in the above equation. The rate coefficients are defined as

$$\mathcal{L}_{nm,kl} = [G(\omega_{nk})N_{nk} - G(\omega_{im})N_{ml}] X_{nk}X_{im} - \delta_{ml} \sum_{j} G(\omega_{jk})N_{jk}X_{nk} + \delta_{nk} \sum_{l} G(\omega_{lj})N_{lk}X_{lk}X_{km}$$

with $N_{nm} = \frac{1}{2}[\coth(\beta \omega_{nm}/2) - 1]$ and $X_{nm} = \langle n | (B^+ + B) | m \rangle$. For the derivation of the master equation, besides the Born and Markov approximations, some more assumptions have been made, which we briefly mention. First, we consider our system and the bath to be initially (at $t = 0$) uncorrelated; i.e., $W(0)_1 = \rho(0)\rho_B(0)$ with $\rho_B(0) = Z_B^{-1}e^{-\beta\mathcal{H}_0}$ and $Z_B$ the partition function of the bath. Further, with the bath consisting of infinite degrees of freedom, we assume the effects of the interaction with the qubit–HO system to dissipate away quickly, such that the bath remains in thermal equilibrium for all times: $W(t)_1 = \rho(t)_1\rho_B(0)$. Besides, an initial slip which occurs due to the sudden coupling of the system to the bath is neglected [2]. And as the last approximation, the Lamb-shift of the oscillation frequencies $\omega_{nm}$ was not taken into account [45].

4.2. Matrix elements

In (37), $X_{nm}$ describes matrix elements of the operator $X = (B + B^\dagger)$ in the qubit–HO eigenbasis. By use of (23a), (23b) and (26) those states were expressed in the basis $\{|jg\rangle; |je\rangle\}$, and we will also calculate the oscillator matrix elements in this basis. For that purpose the operator $\tilde{X} = e^{iS}(B^\dagger + B) e^{-iS}$ is defined. Four different situations can be distinguished. There are matrix elements where neither the oscillator nor the qubit state is changed, namely $\langle jg | \tilde{X} | jg \rangle = -2L_0$ and $\langle je | \tilde{X} | je \rangle = 2L_0$ with $L_0 = \varepsilon g / \Delta b \Omega$. We see that those elements are independent of $j$, the occupation number of the oscillator. Next, we look at the case where a single quantum is emitted or absorbed from the oscillator and get $\langle jg | \tilde{X} | (j+1)g \rangle = \sqrt{J+1}(1+L_{\text{osc}})$ and $\langle je | \tilde{X} | (j+1)e \rangle = \sqrt{J+1}(1-L_{\text{osc}})$ with

$$L_{\text{osc}} = \frac{(2\Delta b + 3\Omega)\Delta b^2}{\Delta b^2(\Delta b + \Omega)^2} g^2.$$  \hspace{1cm} (38)

For a transition within the qubit, we have $\langle jg | \tilde{X} | je \rangle = \Delta_0 g / \Delta b(\Delta b + \Omega) \equiv L_q$. And finally, if the qubit and the oscillator state are changed simultaneously, one obtains $\langle jg | \tilde{X} | (j+1)e \rangle = \sqrt{J+1}L_{q,\text{osc}}^+$ and $\langle je | \tilde{X} | (j+1)g \rangle = \sqrt{J+1}L_{q,\text{osc}}^-$, where

$$L_{q,\text{osc}}^+ = \frac{4\varepsilon \Delta_0}{\Delta b^2(\Delta b + \Omega)(\Delta b + 2\Omega)} g^2 \quad \text{and} \quad L_{q,\text{osc}}^- = \frac{-4\varepsilon \Delta_0}{\Delta b^2(\Delta b - 2\Omega)} g^2.$$  \hspace{1cm} (39)
Comparing the magnitude of the transition terms, we notice that those consisting in changes of the oscillator occupation only are the dominant ones, as they have a part which is of zeroth order in \( g \). Further, for the case in which the qubit is operated at the degeneracy point \( L_0 \) and \( L_{q,osc}^{+/-} \) vanish. With those results we can calculate the matrix elements \( X_{nm} \). They are given in appendix C.

4.3. Dynamics in the dissipative case

Like in section 3.3, we assume the system to be operated at low temperatures and thus take as highest qubit–HO state the eigenstate \( |4\rangle \). For determination of \( P(t) \) the formulae of section 2.2 can be used. Unlike in the non-dissipative case, \( \rho(t) \) is not given anymore by the simple expression (28). Rather we have to solve a system of coupled differential equations, namely (36). To do this analytically, we will follow three different approaches and compare them finally to the numerical solution of (36).

4.3.1. Full secular approximation (FSA). As a first approach, we make the FSA; i.e. we neglect fast rotating terms in (41) and keep only contributions where \( \omega_{nm} - \omega_{kl} \) vanishes. In this way the off-diagonal elements of \( \sigma_{nm} \) are decoupled from the diagonal ones so that

\[
\dot{\sigma}_{nn}(t) = \pi \sum_k L_{nn, kk} \sigma_{kk}(t),
\]

(42)

\[
\dot{\sigma}_{nm}(t) = \pi L_{nm, nm} \sigma_{nm}(t) \quad \text{for } n \neq m.
\]

(43)

The equation for the off-diagonal elements is then

\[
\sigma_{nm}(t) = \sigma_{nm}^0 e^{\pi L_{nm, nm} t},
\]

(44)

which becomes with (40)

\[
\rho_{nm}(t) = \rho_{nm}^0 e^{\pi L_{nm, nm} t} e^{-i\omega_{nm} t}.
\]

(45)

As through the FSA the oscillatory motion of the dynamics is separated from the relaxation one we can divide (13) into two parts,

\[
P(t) = P_{relax}(t) + P_{dephas}(t),
\]

(46)

where \( P_{relax}(t) = \sum_n p_n(t) \) describes the relaxation and \( P_{dephas}(t) = \sum_{n>m} p_{nm}(t) \) the dephasing parts of the dynamics. With (45) the latter takes the form

\[
P_{dephas}(t) = \sum_{n>m} p_{nm}(0) e^{-\Gamma_{nm} t} \cos(\omega_{nm} t)
\]

(47)

with the dephasing rates \( \Gamma_{nm} = -\pi L_{nm, nm} \). Expressions for the dephasing coefficients \( L_{nm, nm} \) can be found in appendix D and the initial conditions \( \rho_{nm}^0 = \sigma_{nm}^0 = \rho_{nm}(0) \) are given by (31). The diagonal elements are more difficult to obtain, as one has to solve a system of coupled differential equations, equation (42). Calculating the corresponding rate coefficients of this
system for the five lowest eigenstates, we find that there are only eight independent ones, namely \( L_{00,11}, L_{00,22}, L_{11,22}, L_{11,33}, L_{11,44}, L_{22,33}, L_{22,44}, L_{33,44} \). They are given by

\[
L_{jk, kk} = 2G(\omega_{jk})N_{jk}X_{jk}^2 \quad \text{with } j < k,
\]  

(48)

where \( j \) and \( k \) adopt the above values. Furthermore, \( L_{00,33}, L_{00,44}, L_{33,00}, \) and \( L_{44,00} \) vanish. The remaining rate coefficients are combinations of the above. We find that

\[
L_{kk,jj} = L_{jj, kk} + 2G(\omega_{jk})X_{jk}^2 = (N_{jk} + 1)2G(\omega_{jk})X_{jk}^2
\]  

(49)

and

\[
L_{00,00} = -L_{11,00} - L_{22,00},
\]

(50a)

\[
L_{11,11} = -L_{00,11} - L_{22,11} - L_{33,11} - L_{44,11},
\]

(50b)

\[
L_{22,22} = -L_{00,22} - L_{11,22} - L_{33,22} - L_{44,22},
\]

(50c)

\[
L_{33,33} = -L_{11,33} - L_{22,33} - L_{44,33},
\]

(50d)

\[
L_{44,44} = -L_{11,44} - L_{22,44} - L_{33,44}.
\]

(50e)

However, the system (42) is still too complicated to be solved analytically. Thus, we invoke a further approximation: we consider the factor \( N_{nm} + 1 \equiv \frac{1}{2} \coth(\hbar \beta \omega_{nm} / 2) + 1 \) with \( n < m \) in (49) and use that \( \lim_{m \to -\infty} \coth(\hbar \beta \omega_{nm} / 2) = -1 \). It depends strongly on the temperature \( \beta \) for which value of \( \omega_{nm} \) this limit is reached approximately. For the parameters we are working with one usually is in the region where \( (N_{nm} + 1) \ll 1 \). Thus, we will neglect in the following terms containing the factor \( (N_{nm} + 1) \). Furthermore, one sees from (27) that \( \omega_{12} \sim g \) and \( \omega_{34} \sim g \). With that \( L_{11,22} = O(g^3) \) and \( L_{33,44} = O(g^3) \) can be neglected. Using (50a)–(50e) the matrix of the system (42) becomes

\[
L_{\text{relax.}} = \begin{pmatrix}
0 & L_{00,11} & L_{00,22} & 0 & 0 \\
0 & -L_{00,11} & 0 & L_{11,33} & L_{11,44} \\
0 & 0 & -L_{00,22} & L_{22,33} & L_{22,44} \\
0 & 0 & 0 & -L_{11,33} - L_{22,33} & 0 \\
0 & 0 & 0 & 0 & -L_{11,44} - L_{22,44}
\end{pmatrix}.
\]

(51)

The eigenvalues and eigenvectors of this matrix and the associated time evolution of the elements \( \sigma_{nm}(t) \) are given in (E.1)–(E.5) of appendix E. Unlike for the dephasing part (47), we cannot extract a simple analytical expression for the relaxation rate as \( P_{\text{relax.}}(t) = \sum_n p_{nn}(t) \) now consists of a sum of several exponential functions, cf (14a) together with (E.1)–E.5). But still we are able to provide an analytical formula for \( P(t) \) using (46).

4.3.2. An ansatz for the long-time dynamics. In order to obtain a simple expression for the relaxation part, we consider the long-time dynamics of the system. In other words, rather than looking at the many relaxation contributions to the populations \( \sigma_{nm}(t) \), we focus on the smallest eigenvalue of the relaxation coefficients, as it will dominate at long times. Further, we consider only the rate matrix associated with the three lowest qubit–HO eigenstates, \( |0\rangle, |1\rangle \) and \( |2\rangle \) in (42) and obtain with (50a)–(50c) that

\[
L_{\text{relax.}} = \begin{pmatrix}
-L_{11,00} - L_{22,00} & L_{00,11} & L_{00,22} \\
L_{11,00} & -L_{00,11} - L_{22,11} & L_{11,22} \\
L_{22,00} & L_{22,11} & -L_{00,22} - L_{11,22}
\end{pmatrix}.
\]

(52)
Figure 3. The relaxation rate \( \Gamma_r \) as it is given in (53) drawn against the oscillator frequency \( \Omega \) (solid line). Used values are \( \varepsilon = 0.5 \Delta_0 \), corresponding to a frequency splitting \( \Delta_b = 1.118 \Delta_0 \), and coupling \( g = 0.18 \Delta_0 \). Moreover, the damping constant is \( \kappa = 0.0154 \) and \( \beta = 10(\hbar \Delta_0)^{-1} \). At resonance (\( \Omega = \Delta_b \)) \( \Gamma_r \) is maximal. For comparison also the second smallest eigenvalue is plotted (dashed line). The inset shows the two eigenvalues close to resonance.

Here, we have not neglected the rate coefficients containing the term \( (N_{nm} + 1) \) and further took \( L_{11,22} \) into account despite of being of third order in \( g \) as such contribution removes the degeneracy between the two lowest eigenvalues at resonance, cf inset in figure 3. The smallest eigenvalue reads

\[
\Gamma_r = -\frac{\pi}{2} \left\{ -\sum_{n \neq m} L_{nn,mm} + \left( \sum_{n \neq m} L_{nn,mm} \right)^2 - 4(L_{00,11}L_{00,22} + L_{11,00}L_{11,22} + L_{00,11}L_{00,22} + L_{11,00}L_{11,22}) \right\}^{1/2}.
\]

(53)

With the system being detuned this expression can be simplified further, namely

\[
\Gamma_r \approx \pi L_{00,22} \quad \text{for} \ \Omega < \Delta_b; \quad \Gamma_r \approx \pi L_{00,11} \quad \text{for} \ \Omega > \Delta_b.
\]

(54)

In figure 3, the relaxation rate \( \Gamma_r \) as obtained from (53) is shown as a function of the oscillator frequency \( \Omega \). Clearly, it is maximal at resonance (\( \Omega = \Delta_b \)), whereas it decays with \( \Omega \) being detuned from the resonance. This effect has already been predicted by Blais et al [12]. As the
qubit is not directly coupled to the bath but rather through the oscillator, the latter being detuned filters out the environmental noise at the qubit transition frequency. Additionally, we show the second smallest eigenvalue of (52). We notice that close to the resonant point \((\Omega = \Delta_b)\) there is an avoided crossing. Finally, we find that

\[
P_{\text{relax}}(t) = (p_0 - p_\infty)e^{-\Gamma_t t} + p_\infty,
\]

where, like in section 3.2, \(p_0 \equiv \sum_n p_{nn}(0)\). For getting \(p_\infty\) we have in principle to find the steady-state solution of (42). Here, we just assume for \(t \to \infty\) a Boltzmann distribution for the qubit–HO system, so that \(\rho_{nn}(\infty) = Z_{\text{QHO}}^{-1}e^{-\beta E_n}\) with \(Z_{\text{QHO}} = \sum_n e^{-\beta E_n}\). Thus,

\[
p_\infty = \sum_n \sum_i \left\{ \cos \Theta \left[ (jg|n\rangle^2 - (je|n\rangle^2) + 2 \sin \Theta (jg|n\rangle\langle je|n\rangle) \right] \rho_{nn}(\infty). \tag{56}\]

The formula for the long-time dynamics is obtained as

\[
P(t) = (p_0 - p_\infty)e^{-\Gamma_t t} + p_\infty + \sum_{n \neq m} p_{nm}(0)e^{-\Gamma_{nm} t} \cos(\omega_{nm} t). \tag{57}\]

To get further insight on the dominant frequencies we evaluate the Fourier transform of (57) according to

\[
F(\omega) = 2 \int_0^\infty dt \cos \omega t P(t), \tag{58}\]

yielding

\[
F(\omega) = 2(p_0 - p_\infty) \frac{\Gamma_t}{\omega^2 + \Gamma_t^2} + 2\pi p_\infty \delta(\omega) + \sum_{n \neq m} p_{nm} \Gamma_{mn} \left[ \frac{1}{\Gamma_{mn}^2 + (\omega_{mn} + \omega)^2} + \frac{1}{\Gamma_{mn}^2 + (\omega_{mn} - \omega)^2} \right]. \tag{59}\]

4.3.3. Partial secular approximation (PSA). An improvement to the FSA is to take into account certain non-vanishing contributions of \(\omega_{nm} - \omega_{kl}\). We have to keep in mind that there are quasi-degenerate levels close to resonance. In our case, the first with second energy level and the third with fourth one build a doublet, meaning that they are close together in energy space. The level spacing is approximately proportional to \(g\) for the former and \(\sqrt{2}g\) for the latter. Because of that and as the transitions from level three and four are less probable, we will in the following only consider the first and second level as being almost degenerate. Taking this into account in (41) we arrive for the diagonal elements at

\[
\dot{\sigma}_{nn}(t) = \pi \sum_k \mathcal{L}_{nn,kk} \sigma_{kk}(t) + \pi \mathcal{L}_{nn,12} \sigma_{12}(t)e^{-i\gamma_{12} t} + \pi \mathcal{L}_{nn,21} \sigma_{21}(t)e^{-i\gamma_{21} t}. \tag{60}\]

A numerical analysis shows that the effect of the last two terms on the right-hand side of the above equation will in the worst case lead to very small wiggles in \(\sigma_{nn}(t)\) and play no role in \(P(t)\). Thus, we finally write

\[
\dot{\sigma}_{nn}(t) \equiv \pi \sum_k \mathcal{L}_{nn,kk} \sigma_{kk}(t), \tag{61}\]

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which is the same equation as we got in the FSA approach. However, the off-diagonal contributions $\sigma_{01}, \sigma_{02}, \sigma_{13}, \sigma_{23}, \sigma_{14}$ and $\sigma_{24}$ have to be examined more carefully. From (41) we find that one has to solve the equations

$$\dot{\rho}_{nm}(t) = (-i\omega_{nm} + \pi L_{nm,nm})\rho_{nm}(t) + \pi L_{nm,jk}\rho_{jk}(t),$$

$$\dot{\rho}_{jk}(t) = \pi L_{jk,nm}\rho_{nm}(t) + (i\omega_{jk} + \pi L_{jk,jk})\rho_{jk}(t)$$

with $\{(nm), (jk)\} = \{(01); (02)\}, \{(13); (23)\}$ or $\{(14); (24)\}$. As the solution one gets

$$\rho_{nm} = \rho_{nm,jk}^{(+)\ d}v_{nm,jk}^{(+)\ d}e^{-i\omega_{nm,jk} t} + \rho_{nm,jk}^{(-)\ d}v_{nm,jk}^{(-)\ d}e^{i\omega_{nm,jk} t},$$

$$\rho_{jk} = \rho_{nm,jk}^{(+)\ d}v_{nm,jk}^{(+)\ d}e^{-i\omega_{nm,jk} t} + \rho_{nm,jk}^{(-)\ d}v_{nm,jk}^{(-)\ d}e^{i\omega_{nm,jk} t}.$$ 

Here, the oscillation frequencies and the decay of the off-diagonal elements are given by

$$\omega_{nm,jk}^{(+)\ d} = \frac{1}{2} \left[ \pi(L_{nm,nm} + L_{jk,jk}) - i(\omega_{nm} + \omega_{jk}) \pm R_{nm,jk} \right]$$

with

$$R_{nm,jk} = \sqrt{\left[ \pi(L_{nm,nm} - L_{jk,jk}) - i(\omega_{nm} - \omega_{jk}) \right]^2 + 4\pi^2 L_{nm,jk}L_{jk,nm}}.$$ 

The amplitudes of the oscillations are given through the coefficients

$$c_{nm,jk}^{(+)\ d} = \frac{e^{\frac{\pi}{2}(L_{nm,nm} - L_{jk,jk}) - i(\omega_{nm} - \omega_{jk}) \pm R_{nm,jk}}}{2R_{nm,jk}}$$

and

$$v_{nm,jk}^{(+)\ d} = \frac{\pi(L_{nm,nm} - L_{jk,jk}) - i(\omega_{nm} - \omega_{jk}) \pm R_{nm,jk}}{\pi}.$$ 

Thus, we have again all the ingredients to calculate analytically the relaxation and dephasing part of (46). For the PSA, we cannot provide a simple expression for the dephasing rates as in the FSA, where we had $\Gamma_{nm} = -\pi L_{nm,nm}$. As one can see from (64) and (65), $\rho_{01}$ and $\rho_{02}$ are a mixture of contributions decaying with Re$\{\lambda_{01,02}^{(+)\ d}\}$ and Re$\{\lambda_{01,02}^{(-)\ d}\}$. Similar to our findings for the relaxation rate, also here the smallest eigenvalue will dominate the dephasing behaviour. From the right graph in figure 4, we find that this is Re$\{\lambda_{01,02}^{(+)}\} \equiv \Gamma_1^{(+)\ d}$ and Re$\{\lambda_{01,02}^{(-)\ d}\} \equiv \Gamma_1^{(-)\ d}$. Comparing it with the dephasing rates, we got using the FSA, left graph in figure 4, we see that for negative detuning ($\Omega < \Delta_b$) the rate $\Gamma_0^{(-)\ d}$ approximates $\Gamma_1^{(-)\ d}$, whereas for positive detuning ($\Omega > \Delta_b$) this is done by $\Gamma_0^{(+)} = -\pi \lambda_{01,01}^{(+)}$. In the FSA, $\Gamma_0^{(+)}$ and $\Gamma_1^{(+)}$ correspond to the frequencies $\omega_{10}$ and $\omega_{20}$, respectively. In the PSA, the frequency $\omega_{12}^{(+)} \equiv \text{Im}\{\lambda_{01,02}^{(+)}\}$ is given by $\omega_{12}^{(+)} = \omega_{20}$ for $\Omega < \Delta_b$ and $\omega_{12}^{(+)} = \omega_{10}$ for $\Omega > \Delta_b$. Hence, for negative detuning oscillations with frequency $\omega_{20}$ will dominate the dynamics, while those with $\omega_{10}$ will almost vanish. For positive detuning, it is the other way round. In (64) and (65), this behaviour is reflected by the coefficients $c_{nm,jk}^{(+)\ d}$ and $v_{nm,jk}^{(+)\ d}$. Around resonance ($\Omega \approx \Delta_b$) the PSA tells us by (64) and (65) that the dephasing rates and frequencies are a mixture of $\Gamma_{01}$ and $\Gamma_{02}$, or $\omega_{10}$ and $\omega_{20}$, respectively. From the left graph in figure 4, one notices further that the FSA rate $\Gamma_0^{(+)\ d}$ grows linearly with $\Omega$ for positive detuning. However, as the weight of the corresponding frequency $\omega_{20}$ will be almost zero, $\Gamma_0^{(+)\ d}$ will give no relevant contribution to $P_{\text{dephas}}(t)$ in this regime but the dephasing will rather be associated with the FSA rate $\Gamma_{01}$. Hence, out of resonance the FSA will still fairly well describe the dynamics of $P(t)$. Comparing the expressions for $\mathcal{L}_{01,01}$ and $\mathcal{L}_{02,02}$ given in appendix D by (D.1) and (D.2)

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Figure 4. Comparison between the dephasing rates of the two dominant frequencies as they are obtained using the FSA or the PSA, respectively. On the left: the FSA rates $\Gamma_{01} \equiv -\pi \mathcal{L}_{01,01}$ (dashed red line) and $\Gamma_{02} \equiv -\pi \mathcal{L}_{02,02}$ (solid black line). On the right: the real part of $\lambda_{01,02}^{(+)}$ (red dashed line) and $\lambda_{01,02}^{(-)}$ (black solid line) as given by (66) is shown. The rate dominating the dephasing behaviour is defined as $\Gamma_{12}^{(+)} \equiv \text{Re}\{\lambda_{01,02}^{(+)}\}$. For $\Omega < \Delta_0$, we see that $\Gamma_{12}^{(+)}$ is approximated by the FSA rate $\Gamma_{02}$, while for $\Omega > \Delta_0$ by $\Gamma_{01}$. Used values are $\varepsilon = 0$, $g = 0.18$, $\kappa = 0.0154$ and $\beta = 10(\hbar\Delta_0)^{-1}$.

with the approximative expressions for the relaxation rate at positive and negative detuning (54), we see that for zero bias ($\varepsilon = 0$) the PSA dephasing rate is equal to $\Gamma_i/2$. For a biased system, an additional term is added depending on the spectral density of the bath at $\omega = 0$. In figure 5, we compare the three analytical solutions described above to the numerical solution of the master equation for the case of an unbiased TLS being at resonance with the oscillator. Concerning both the dynamics of $P(t)$ and its Fourier spectrum, we see a good agreement between the different solutions. The one being closest to the numerical solution is the PSA solution. We also want to mention that going to stronger damping $\kappa$, the FSA results start to show deviations from the numerical solution. Here, one should use the PSA only. However, for the parameter regime used in the following, we will mainly apply (57) due to its simple, analytical form.

5. Discussion of the results

Having solved the master equation (36) analytically and numerically, we can examine the dynamics of the system and its Fourier transform for different situations. First, we will look at a qubit operated at the degeneracy point ($\varepsilon = 0$) being in and out of resonance with the oscillator. Then, we will concentrate on the biased qubit in the same regime of parameters.

5.1. The unbiased qubit

For unbiased qubits, we can compare our predictions with the analytical results obtained in [31] by starting from a spin-boson model with the effective spectral density (10). In [31], a so-called weak damping approximation (WDA) based on the NIBA is applied. The WDA allows a...
non-perturbative treatment of the coupling between the TLS and HO and hence can reproduce the occurrence of two dominating frequencies as expected e.g. from exact QUAPI calculations \([27]\). The NIBA, and hence the WDA, however, become not reliable for a biased TLS. We find that the overall agreement between our approach and the WDA is very good. However, in the WDA solution the frequencies are slightly shifted compared to the ones obtained from our master equation. This may result from the perturbative expansion we have performed with respect to \(g\) by applying the Van Vleck perturbation theory.

First, we look at the resonant case shown in figure 6. In agreement with previous works \([27, 31]\), we find that the dynamics is dominated by two frequencies corresponding to \(\omega_{10}\) and \(\omega_{20}\) with separation being approximately \(2g\). The weight of the latter is a bit larger. The reason for the bigger weight is that at resonance \((\Omega = \Delta_0)\) the qubit–HO eigenstate \(|j\rangle\) is not a symmetric superposition of the states \(|j, e\rangle\) and \(|j + 1, g\rangle\) unlike it is predicted by the Janyes–Cummings model (cf e.g. \([12]\)). We notice that the two unequal peaks have indeed been experimentally observed in \([13]\) (see figure 4(b) therein). Considering the states \(|1\rangle_{\text{eff}}\) and \(|2\rangle_{\text{eff}}\) in \((23a)\) and \((23b)\), one already sees that for a symmetric superposition of these states we need that \(\delta_0\) vanishes or that \(\Omega \equiv [(\Delta_0^4 + 2g^2\Delta_0^2)/\Delta_0^2]^{1/2}\) (cf equation \((78)\)). Besides, in order to get the qubit–HO eigenstates, one still has to perform the Van Vleck transformation, which adds contributions to \(|1\rangle\) and \(|2\rangle\) from states corresponding to oscillator levels higher than \(j = 1\). Thus, our system behaves for \(\Omega = \Delta_0\) as being negatively detuned, which means that the peak belonging to the higher frequency dominates, as we will show below. Slightly increasing \(\Omega\) will give a stronger weight to the peak at \(\omega_{10}\). This effect is not very pronounced for the non-dissipative dynamics of the unbiased qubit (figure 2), as there the two frequencies are still almost equally weighted. Looking however at the Fourier transform of the dissipative dynamics \((59)\),
Figure 6. Dynamics of the population difference $P(t)$ (left-hand side) and its Fourier transform $F(\omega)$ (right-hand side) for an unbiased TLS being in resonance with the oscillator ($\Omega = \Delta_0$). The numerical solution of the master equation (black solid line) is compared with the analytical expressions (57) and (59) (red dashed line) and the WDA from [31] (green dotted-dashed line). The parameters are $\varepsilon = 0$, $\Omega = \Delta_0$, $g = 0.18\Delta_0$, $\kappa = 0.0154$ and $\beta = 10(\hbar\Delta_0)^{-1}$. From the Fourier transform, one sees that two frequencies are dominating the dynamics. The separation of those two peaks is approximately $2g$. The non-dissipative dynamics is shown for comparison in figure 2.

Next, we consider in figure 7 the case of negative detuning, where $\Omega < \Delta_0$. No matter which approach one is looking at, clearly the frequency $\omega_{20}$ is dominating. Furthermore, paying attention to the timescale of the dynamics, one notices that the relaxation time is enhanced compared with the one we found for the resonant system. This behaviour was already explained by the formula (53) for the relaxation rate. Again, the numerical and the solution obtained by using the long-time ansatz in section 4.3.2 agree quite well with each other, whereas the amplitude of the oscillation with frequency $\omega_{20}$ is stronger in the WDA approach. Also remarkable is the fact that looking at the Fourier transform in figure 7, one sees in the inset already small contributions of the higher oscillator levels. The transitions corresponding to $\omega_{24}$ and $\omega_{23}$ give rise to small additional peaks, while the contributions of $\omega_{13}$ and $\omega_{14}$ are negatively weighted and cause dips. The WDA approach does not show these additional contributions. They are, however, confirmed by the numerical QUAPI calculations in [27] (see figure 2 therein). In the case of positive detuning ($\Omega > \Delta_0$) shown in figure 8, we find a quite good agreement between all three approaches. Also for positive detuning the relaxation time is enhanced compared to the resonant case. Contrary to the negatively detuned situation the additional peaks have vanished. Besides, now the frequency $\omega_{10}$ is dominating the dynamics. This behaviour, namely that for negative detuning $\omega_{20}$ and for positive detuning $\omega_{10}$ is dominating, was already found in [27].

We will briefly explain how one can explain this observation physically. For this we look at figure 9. For a detuned system ($\Omega \neq \Delta_b$), the qubit–HO eigenstates are not symmetric...
Figure 7. Dynamics of $P(t)$ and its Fourier transform $F(\omega)$ for negative detuning ($\Omega < \Delta_0$) and for $\varepsilon = 0$. Same parameters as in figure 6 are used except that now $\Omega = 0.75\Delta_0$. The frequency $\omega_{20}$ dominates the dynamics. The inset on the right graph shows a zoom into the Fourier transform. The numerical solution and the analytical expression (59) exhibit besides the main peaks at $\omega_{10}$ and $\omega_{20}$ two additional peaks, corresponding to the frequencies $\omega_{24}$ (between the two main peaks) and $\omega_{23}$ (on the left of the first main peak). The two dips come from $\omega_{13}$ and $\omega_{14}$.

Figure 8. Dynamics of $P(t)$ and its Fourier transform $F(\omega)$ for positive detuning ($\Omega > \Delta_0$), for $\varepsilon = 0$ and $\Omega = 1.5\Delta_0$. The peak at $\omega_{10}$ dominates. No additional peaks are found. A very good agreement between all approaches discussed in the text is found. Remaining parameters are as in figure 6.

superpositions of the states $|jg\rangle$ and $|je\rangle$. They rather asymptotically approach the eigenstates of the uncoupled qubit–HO Hamiltonian. In figure 1, we see that for a negatively detuned system (line a) the qubit–HO eigenstate $|2j + 1\rangle$ approaches the state $|(j + 1)g\rangle$, whereas the main contribution to the state $|2j + 2\rangle$ will come from the state $|je\rangle$. From the left diagram in figure 9, we see that the state $|2\rangle$ is energetically higher than the state $|1\rangle$. However, due to the Boltzmann distributed occupation of the oscillator, the state $|0e\rangle$ will be more populated than
the state $|1g\rangle$ and consequently also $|2\rangle$ will exhibit a larger population than $|1\rangle$, as the latter only feels a small contribution from the state $|0e\rangle$. Thus, transitions from $|2\rangle$ to the ground state are more likely to occur than those from $|1\rangle$ to the ground state. This explains the dominance of $\omega_{20}$ in figures 7 and 11. In this case, the frequencies $\omega_{20} \approx \Delta_b$ and $\omega_{10} \approx \Omega$. As far as not excluded by selection rules, minor peaks from transitions to the levels lying in between can be also seen.

For positive detuning (line c in figure 1) $|2j+1\rangle$ approaches $|je\rangle$, while $|2j+2\rangle$ is close to $|(j+1)g\rangle$. From the right graph in figure 9, we see that the state $|1\rangle$, being lowest in energy apart from the ground state, is now also more likely to be occupied than $|2\rangle$. Therefore, as confirmed by figures 8 and 12, the frequency $\omega_{10}$ is dominating whereas $\omega_{20}$ is represented only by a small peak in the Fourier spectrum. Furthermore, as there are no additional energy levels between the state $|1\rangle$, which is most probably to be populated, and the ground level, other transitions than those corresponding to $\omega_{10}$ or $\omega_{20}$ are very unlikely to occur. In figure 12, the dip corresponding to $\omega_{21}$ appears only very faintly.

### 5.2. The biased qubit

We will now examine a qubit being operated at finite bias. We consider the case $\varepsilon > 0$. For negative bias-offset, the behaviour is analogous. Again three different situations are taken into account: the qubit being in resonance with the oscillator ($\Delta_b = \Omega$), negative ($\Omega < \Delta_b$) and positive ($\Omega > \Delta_b$) detuning.

For the resonant case ($\Omega = \Delta_b$) depicted in figure 10, we see a similar behaviour as for the unbiased qubit. Again two frequencies, $\omega_{10}$ and $\omega_{20}$, are dominating the dynamics. Left of the peak at $\omega_{10}$ a small dip can be found in the Fourier spectrum. This corresponds to the transition $\omega_{21}$. For infinite time, the dynamics relaxes to an equilibrium value which is nonzero in contrast to the unbiased qubit. This can be seen in the Fourier spectrum through a relaxation peak at $\omega = 0$. The peak arises because of the term

$$2(p_0 - p_\infty) \frac{\Gamma_r}{\omega^2 + \Gamma_r^2} + 2\pi p_\infty \delta(\omega)$$

in (59). The first part of this sum gives rise to the negative shift of this peak. The reason that for the analytical solution the peak is not as strongly shifted as for the numerical one is technical: in
Figure 10. Dynamics of $P(t)$ and its Fourier transform $F(\omega)$ for the biased qubit being in resonance with the oscillator. Here, $\varepsilon = 0.5\Delta_0$ and $\Omega = \Delta_b$. The remaining parameters are the same as for the unbiased qubit. In the Fourier spectrum, the frequencies $\omega_{10}$ and $\omega_{20}$ dominate. At frequency $\omega_{21}$, a small dip can be seen. At $\omega = 0$, the spectrum exhibits a relaxation peak.

Figure 11. Dynamics of $P(t)$ and its Fourier transform $F(\omega)$ for negative detuning ($\Omega < \Delta_b$) with $\Omega = 0.9$ and $\varepsilon = 0.5$. Next to the numerical solution (black solid curve) of the full master equation and the FSA solution (57) and (59) (red dashed curve), also the improved FSA solution of (42) and (43) (green dotted-dashed curve) are shown. The dynamics is dominated by $\omega_{20}$. The peak at $\omega_{10}$ is much weaker. Like for the resonant, biased qubit, a dip is found at $\omega_{21}$ and a relaxation peak at $\omega = 0$.

In order to plot the delta function in (70) we gave it a finite width, which suppresses the negative contribution of the first term in (70). Like for the unbiased qubit the highest energy level playing a role for the dynamics is $E_2$; i.e. only the ground and first excited levels of the oscillator are of importance. In figure 11, the dynamics and its Fourier transform for a negatively detuned qubit–oscillator system with $\varepsilon \neq 0$ are shown. Like for the unbiased case, detuning gives rise to longer relaxation times for the qubit. Also in agreement with the unbiased case is the dominance of the frequency $\omega_{20}$. We see that for small $t$ the long-time solution (57) slightly overestimates...
Figure 12. Dynamics and Fourier transform for positive detuning ($\Omega > \Delta_b$) for $
abla = 1.5\Delta_0$ and $\varepsilon = 0.5\Delta_0$. Like in figure 11, three different approaches are compared. In all three cases the frequency $\omega_1$ dominates. The maxima of the oscillations and underestimates its minima. Furthermore, we get here the unphysical situation that the maximum of the third oscillation in $P(t)$ exceeds the value of one. The reason for this behaviour is that, by construction, we underestimate with (57) the relaxation at short times. As for certain parameters the term $(p_0 - p_\infty)$ in (57) can become negative, it increases too fast towards the equilibrium and thus gives rise to the observed deviations in the short time behaviour. On a longer timescale, both graphs agree quite well. For the case of positive detuning ($\Omega > \Delta_b$), which is presented in figure 12, the upward shift of the dynamics obtained from (57) and (59) compared with the numerical graph of $P(t)$ at small times is even stronger. To visualize that it is not a failure of the FSA approach, we show in figures 11 and 12 additionally the analytical FSA solution of (42) and (43) calculated in section 4.3.1. The latter agrees very well with the numerical solution. At long timescales and for the Fourier spectrum all three approaches match with each other very well.

To conclude this section, we want to mention that all the results found both for the unbiased and the biased qubit confirm the numerical QUAPI results in [27].

5.3. Symmetrized correlation function

So far we have always considered the qubit for certain values of $\varepsilon$ and finite or zero detuning. In this section, we fix the oscillator frequency at $\Omega = \Delta_0$. That means that an unbiased qubit will be at resonance with the oscillator. Changing the bias to positive or negative values will always lead to negative detuning, as $\Delta_b \geq \Delta_0$. Figure 13 shows a density plot of the Fourier transform of the symmetrized correlation function against the bias of the qubit and the Fourier frequency $\omega$. We consider this correlation function rather than $P(t)$, as it is symmetric in the bias $\varepsilon$. The symmetrized correlation function is defined as follows [2]:

$$S(t) = \frac{1}{2} (\sigma_z(t)\sigma_z(0) + \sigma_z(0)\sigma_z(t)) - p_\infty^2,$$

(71)

where $\sigma_z(t) = e^{i\hat{H} t / \hbar} \sigma_z e^{-i\hat{H} t / \hbar}$. Expressed in terms of the population difference $P(t)$ this becomes,

$$S(t) = P_s(t) + p_\infty (P_a(t) - p_\infty),$$

(72)
Figure 13. Fourier transform of the symmetrized correlation function plotted versus Fourier frequency $\omega$ and qubit bias $\epsilon$. In the left-hand graph $S(\omega)$ is plotted in linear scale, in the right-hand graph $|S(\omega)|$ in logarithmic scale. The parameters are: $\Omega = \Delta_0$, $g = 0.18\Delta_0$, $\kappa = 0.0154$ and $\beta = 10(\hbar\Delta_0)^{-1}$. The white dashed, horizontal line indicates the oscillator frequency $\omega = \Omega$. The other two dashed white lines correspond to $\omega = \Delta_b$ and $\omega = \Delta_b - \Omega$.

with $P_s(t)$ and $P_a(t)$ being symmetric and antisymmetric in $\epsilon$ and $P(t) = P_s(t) + P_a(t)$. The Fourier transform of $S(t)$ is defined as

$$S(\omega) = 2 \int_0^\infty dt \cos(\omega t)S(t).$$

(73)

Considering now figure 13, we see that for any bias the spectrum is dominated by two frequencies, namely $\omega_{10}$ and $\omega_{20}$. Detuning the system $\omega_{20}$ gets more and more important, as we could already observe in the two previous sections for the positively detuned systems. Furthermore, the peaks are shifted to higher frequency values and at $\omega = 0$ the relaxation peak occurs. We want to compare these results to a circuit QED experiment performed by Wallraff et al [13]. There the qubit is realized by a CPB, which is coupled to a superconducting transmission line resonator. The properties of the system are determined by probing the resonator spectroscopically. The amplitude of a microwave probe beam transmitted through the resonator is measured versus the probe frequency and the gate charge of the CPB (see figure 4 in [13]). Via the gate charge the qubit can be detuned in situ from the degeneracy point. The frequency of the resonator is chosen in such a way that it is in resonance with a qubit being operated at the degeneracy point. For the resonant case, two dominating frequencies, being almost equally weighted and symmetrically positioned around the cavity frequency, are observed. Going away from the degeneracy point the system becomes detuned and the frequency of the cavity dominates. The behaviour we observe in figure 13 is similar. However, as we are looking at the dynamics of the qubit, it corresponds to a spectroscopic measurement on the TLS rather than on the oscillator. As explained above the two lowest excited states of the coupled TLS–HO system, namely $|1\rangle$ and $|2\rangle$, evolve from an almost symmetric superposition of basis states $\{|jg\rangle, |je\rangle\}$ at resonance ($\epsilon = 0$) to the states $|1g\rangle$ and $|0e\rangle$ (cf the left graph in figure 9). For $\epsilon = 0$, the two peaks of the Rabi splitting are observed. For $\epsilon \neq 0$, which
means negative detuning in this case, the peak with the lower frequency corresponding to \( \omega_{10} \) approaches more and more the frequency \( \Omega \) of the oscillator, as the state \( |1\rangle \) becomes \( |1g\rangle \) for large detuning and then \( \hbar \omega_{10} \approx E_{\langle 1g \rangle} - E_{\langle 0g \rangle} = \hbar \Omega \). Furthermore, the transition peak at \( \omega_{10} \) gets weaker as also the occupation probability of \( |1\rangle \) decreases. At \( \varepsilon \approx \pm 0.8 \Delta_0 \), the symmetrized correlation function vanishes at \( \omega_{10} \) and increases again for higher values of \( |\varepsilon| \). Here, the amplitude \( p_{10} \) in \( P(t) \) changes its sign. In contrast the peak at \( \omega_{20} \) becomes stronger with the detuning and approaches more and more the qubit splitting energy \( \hbar \Delta_b \), as \( |2\rangle \) approaches \( |0e\rangle \) and then \( \hbar \omega_{20} \approx E_{\langle 0e \rangle} - E_{\langle 0g \rangle} = \hbar \Delta_b \). Additionally, looking at the logarithmic plot one sees around \( \omega = 0.4 \Delta_0 \) a peak appearing, which corresponds to the frequency \( \omega_{21} \) and is forbidden at \( \varepsilon = 0 \). For large detuning, it arises from transitions from \( |0e\rangle \) to \( |1g\rangle \) and therefore has the value \( \omega_{21} \approx \Delta_b - \Omega \). The amplitude of this peak is very small compared with the peaks at \( \omega_{10} \) and \( \omega_{20} \) and is not resolved in the experiment of Wallraff et al.

6. Comparison with the Jaynes–Cummings model

The Van Vleck perturbation theory enabled us to find approximately the eigenstates and eigenenergies of the full Hamiltonian of the TLS–HO system without performing a RWA. Using those eigenstates and eigenenergies in a Born–Markov master equation, we could calculate the dynamics of such a system under the influence of an environmental bath. In the following we will show how the results change if we neglect counter-rotating terms in the TLS–HO Hamiltonian (16) for \( \varepsilon = 0 \). For this, we rewrite the interaction part in (16) as

\[
\tilde{H}_{\text{int}} = \tilde{H}_{\text{int}}^R + \tilde{H}_{\text{int}}^{CR} = -\hbar g(\tilde{\sigma}^+ B + \tilde{\sigma}^- B^\dagger) - \hbar g(\tilde{\sigma}^- B + \tilde{\sigma}^+ B^\dagger),
\]

where we identified with \( \tilde{H}_{\text{int}}^R \) and \( \tilde{H}_{\text{int}}^{CR} \) a rotating and counter-rotating part of \( \tilde{H}_{\text{int}} \), respectively, and introduced the two-level transition operators \( \tilde{\sigma}^\pm = \frac{1}{2}(\tilde{\sigma}_x \pm i\tilde{\sigma}_y) \). Neglecting the counter-rotating part \( \tilde{H}_{\text{int}}^{CR} \) in \( \tilde{H}_{\text{HO}} \) leads to the Jaynes–Cummings Hamiltonian

\[
\tilde{H}_{JC} = -\frac{\hbar \Delta_b}{2} \tilde{\sigma}_z + \hbar \Omega B^\dagger B - \hbar g(\tilde{\sigma}^- B + \tilde{\sigma}^+ B^\dagger).
\]

This Hamiltonian can be diagonalized exactly and its eigenstate and eigenvalues can, for example, be found in [46]. In order to see the effect of not taking into account the counter-rotating terms, we diagonalize \( \tilde{H}_{JC} \) using the Van Vleck perturbation theory. Looking at the formula for the effective Hamiltonian (B.6) in appendix B and keeping in mind that we set \( \varepsilon \) to zero, we see that the second-order contributions in \( g \) vanish neglecting \( \tilde{H}_{\text{CR}}^\dagger \), i.e. \( W_1, W_0 \) are zero in (21). Considering further the transformation matrix \( S \), equations (B.4) and (B.5) in appendix B show that \( S = 0 \) for \( \tilde{H}_{\text{CR}} = 0 \). Thus, with (17) we find that for the Jaynes–Cummings model \( \tilde{H}_{\text{eff}} \) is identical to \( \tilde{H}_{JC} \) and therefore the eigenstates of \( \tilde{H}_{\text{eff}} \) are simultaneously eigenstates of \( \tilde{H}_{JC} \). Consequently, one can determine from (22)–(24) the eigenstates and eigenenergies of \( \tilde{H}_{JC} \). The energy of the ground state \( |0\rangle^{JC} = |0g\rangle^{JC} \) is \( E_{\langle 0 \rangle}^{JC} = -\hbar \Delta_b/2 \). For the higher states, we get

\[
|2j + 1\rangle^{JC} = \cos \left( \frac{\alpha_j^{JC}}{2} \right) |(j + 1)g\rangle + \sin \left( \frac{\alpha_j^{JC}}{2} \right) |je\rangle,
\]

\[
|2j + 2\rangle^{JC} = -\sin \left( \frac{\alpha_j^{JC}}{2} \right) |(j + 1)g\rangle + \cos \left( \frac{\alpha_j^{JC}}{2} \right) |je\rangle.
\]
corresponding to the eigenenergies
\[
E_{{2j+1/2j+2}} = \hbar \left[ \left( j + \frac{1}{2} \right) \Omega + \frac{\delta_{JC}}{2 \cos \alpha^C_j} \right] = \hbar \left[ \left( j + \frac{1}{2} \right) \Omega + \frac{1}{2} \sqrt{\delta_{JC}^2 + 4(j + 1)|\Delta|^2} \right].
\]

with \( \delta_{JC} = \Delta_b - \Omega \) and \( \tan \alpha^C_j = 2\sqrt{\frac{\Omega}{\Delta_b}} |\Delta|/\delta_{JC} \). Comparing these eigenstates and eigenenergies to the ones found for \( \tilde{\mathcal{H}}_{QHO} \), (23a), (23b) and (26), we see that the counter-rotating terms yield second-order corrections in \( g \) not present in the Jaynes–Cummings Hamiltonian. These corrections give rise to a very prominent effect concerning the resonance condition between TLS and HO. From \( \delta_{JC} \) we find the TLS being in resonance with the oscillator for \( \Omega = \Delta_b \).

Considering \( \delta_j \) in (25) this resonance condition is shifted to
\[
\Omega = \Delta_b \sqrt{1 + 2(j + 1) \frac{\Delta_p^2}{\Delta_b^2} g^2} \approx \Delta_b \left[ 1 + \frac{1}{2} (2j + 1) \frac{\Delta_p^2}{\Delta_b^2} g^2 + O(g^3) \right].
\]

This second-order correction to the resonance frequency due to counter-rotating terms is known as the Bloch–Siegert shift [43]. The eigenstates (76a) and (76b) are always a superposition of two basis states of the unperturbed system. This is similar to the case of eigenstates (23a) and (23b) of the effective Hamiltonian (17). However, in order to find the eigenstates \( |n\rangle \) of \( \tilde{\mathcal{H}}_{QHO} \) we had to apply the transformation \( \exp(-i\mathcal{S}) \) on the effective eigenstates so that \( |n\rangle \) is in the end a superposition of several states of the basis \( \{|jg\rangle; |je\rangle\} \).

To calculate the reduced density matrix of the qubit–HO system described by \( \tilde{\mathcal{H}}_{JC} \) and taking into account the influence of an environmental oscillator bath we can again use the Born–Markov master equation (36). We just have to use (76a) and (76b) as basis states and the corresponding eigenenergies. For the population difference, \( P(t) \), we apply (13), which becomes for \( \varepsilon = 0 \)
\[
P(t) = \sum_n p_{nn}(t) + \sum_{n \neq m} p_{nm}(t)
\]
\[
= \sum_n \sum_j 2\langle jg|n \rangle \langle je|n \rangle \rho_{nn}(t) + 2 \sum_{n \neq m} \sum_j \left[ \langle je|n \rangle \langle mj|g \rangle + \langle je|m \rangle \langle nj|g \rangle \right] \text{Re} \{ \rho_{nm}(t) \}.
\]

(79)

6.1. Selection rules

Before doing a qualitative comparison between the results obtained from the original Hamiltonian \( \tilde{\mathcal{H}}_{QHO} \) and the simplified form \( \tilde{\mathcal{H}}_{JC} \), we want to analyse which transitions between the different eigenstates of \( \tilde{\mathcal{H}}_{JC} \) yield contributions to \( P(t) \). For this it is helpful to rewrite (76a) and (76b). In the following, we neglect the upper index JC denoting an eigenstate of \( \tilde{\mathcal{H}}_{JC} \). For the state \( |n\rangle \), we have three possibilities: the first one corresponds to \( n = 0 \). In this case, the only non-vanishing component of \( |0\rangle \) is \( \langle 0g|0 \rangle \). Second, \( n \) can be an even number, which means, expressed in terms of oscillator quanta, that \( n = 2j + 2 \). Then
\[
|n_{ev} \rangle = -\sin(\alpha_{(n-2)/2} \sqrt{\frac{n}{2}}) g + \cos(\alpha_{(n-2)/2} \sqrt{\frac{n}{2}}) \left( \frac{n - 2}{2} \right) e.
\]

And third for an odd state \( n = 2j + 1 \), we find
\[
|n_{od} \rangle = \cos(\alpha_{(n-1)/2} \sqrt{\frac{n}{2}}) \left( \frac{n + 1}{2} \right) g + \sin(\alpha_{(n-1)/2} \sqrt{\frac{n}{2}}) \left( \frac{n - 1}{2} \right) e.
\]

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It is quite easy to see that the part $p_{nm}(t)$ in (79) vanishes for any $n$. That means that the diagonal elements of the reduced density matrix yield no contributions to $P(t)$ for $\varepsilon = 0$ and the equilibrium value of the dynamics will be also zero. Not so easy to see are the combinations of $n$ and $m$ yielding contributions to the off-diagonal part $p_{nm}(t)$.

Considering transitions to the ground state ($m = 0$), we find using that $\langle 0g | 0 \rangle = 1$ that
\[
p_{n_{ev}0} = 2\langle 0e | n_{ev} \rangle \text{Re}\{\rho_{n_{ev}0}(t)\}
\]
and that
\[
p_{n_{od}0} = 2\langle 0e | n_{od} \rangle \text{Re}\{\rho_{n_{od}0}(t)\}.
\]

With (80) and (81) these elements are nonzero only if $n = 1$ or $n = 2$. For the more general case with $n \neq m$ and both being different from zero, we have to investigate products of components like $\langle je | n ev \rangle \langle m | j g \rangle$. For $p_{n_{ev}m_{ev}}(t)$, we find that
\[
\langle je | n_{ev} \rangle \langle m_{ev} | j g \rangle \neq 0 \quad \text{if} \quad j = \frac{n_{ev} - 2}{2} \quad \text{and} \quad j = \frac{m_{ev}}{2},
\]
and that
\[
\langle je | m_{ev} \rangle \langle n_{ev} | j g \rangle \neq 0 \quad \text{if} \quad j = \frac{m_{ev} - 2}{2} \quad \text{and} \quad j = \frac{n_{ev}}{2},
\]
so that
\[
p_{n_{ev}m_{ev}}(t) \neq 0 \quad \text{if} \quad |n_{ev} - m_{ev}| = 2.
\]

For the case of transitions between odd states, one gets that
\[
\langle je | n_{od} \rangle \langle m_{od} | j g \rangle \neq 0 \quad \text{if} \quad j = \frac{n_{od} - 1}{2} \quad \text{and} \quad j = \frac{m_{od} + 1}{2},
\]
and similarly under exchange of $n_{od}$ and $m_{od}$, so that
\[
p_{n_{od}m_{od}}(t) \neq 0 \quad \text{if} \quad |n_{od} - m_{od}| = 2.
\]

For transitions from an even to an odd state and vice versa, we have to pay attention to the fact that
\[
\langle je | n_{ev} \rangle \langle m_{od} | j g \rangle \neq 0 \quad \text{if} \quad j = \frac{n_{ev} - 2}{2} \quad \text{and} \quad j = \frac{m_{od} + 1}{2},
\]
which yields the selection rule $n_{ev} - m_{od} = 3$. Further,
\[
\langle je | m_{od} \rangle \langle n_{ev} | j g \rangle \neq 0 \quad \text{if} \quad j = \frac{m_{od} - 1}{2} \quad \text{and} \quad j = \frac{n_{ev}}{2},
\]
yielding $m_{od} - n_{ev} = 1$. To sum up: $p_{nm}(t)$ is nonzero if one of the three following cases is valid: $|n_{ev} - m_{ev}| = 2$, $|n_{od} - m_{od}| = 2$, $n_{ev} - m_{od} = 3$ or $m_{od} - n_{ev} = 1$. The allowed transitions are shown in figure 14. One sees that transitions between almost degenerate levels are forbidden. We have also found this behaviour in section 3.3 for the non-dissipative dynamics resulting from $\hat{H}_{\text{QHO}}$.

6.2. Comparison of the two models

In the following, we compare the numerical solution of the Born-Markov master equation originating from the Jaynes–Cummings Hamiltonian with the solution using the eigenstates of the full Hamiltonian $\hat{H}_{\text{QHO}}$, which we found by applying the Van Vleck perturbation theory. The fixed parameters we use are in units of $\Delta_0$: $\varepsilon = 0$, $g = 0.18$, $\kappa = 0.0154$ and $\beta = 10$. The oscillator frequency $\Omega$ is varied. For all the three possible cases (positive, negative and zero detuning) one notices from figures 15–17 that the Jaynes–Cummings approach underestimates
Figure 14. Possible transitions between the first six eigenstates of the Jaynes–Cummings Hamiltonian are indicated by the red arrows. Transitions between almost degenerate levels are forbidden at zero bias ($\varepsilon = 0$).

Figure 15. Dynamics $P(t)$ of the population difference and its Fourier transform $F(\omega)$ for positive detuning ($\Omega = 1.5\Delta_0$). The parameters are in units of $\Delta_0$: $\varepsilon = 0$, $g = 0.18$, $\kappa = 0.0154$ and $\beta = 10$. The red dashed line shows the solution obtained numerically from the master equation using the eigenstates and eigenenergies from the full Hamiltonian $H_{QHO}$. The solid line shows the results obtained from the Jaynes–Cummings Hamiltonian.

The dephasing rate $\Gamma_{10}$ (means a larger peak at frequency $\omega_{10}$) and overestimates the rate $\Gamma_{20}$ (smaller peak at $\omega_{20}$) compared with the approach with the full Hamiltonian.

The case of positive detuning ($\Omega > \Delta_0$) is shown in figure 15. As here the dynamics is dominated by the frequency $\omega_{10}$, the equilibrium value is reached on a too long timescale using the Jaynes–Cummings Hamiltonian. On the contrary, for negative detuning ($\Omega < \Delta_0$), which is shown in figure 16 and where $\omega_{20}$ dominates, the equilibrium value is reached too...
Figure 16. Dynamics $P(t)$ of the population difference and its Fourier transform $F(\omega)$ for negative detuning ($\Omega = 0.75\Delta_0$). The remaining parameters are the same as in figure 15. The red dashed line shows the solution obtained numerically from the master equation using the eigenstates and eigenenergies from the full Hamiltonian $\mathcal{H}_{QHO}$. The solid line shows the results obtained from the Jaynes–Cummings Hamiltonian.

Figure 17. Dynamics $P(t)$ of the population difference and its Fourier transform $F(\omega)$ for the resonant case ($\Omega = \Delta_0$). The remaining parameters are the same as in figure 15. The red dashed line shows the solution obtained numerically from the master equation using the eigenstates and eigenenergies from the full Hamiltonian $\mathcal{H}_{QHO}$. The solid line shows the results obtained from the Jaynes–Cummings Hamiltonian.

fast within the Jaynes–Cummings approach. Furthermore, considering the graph of the Fourier transform we find that small contributions which come from higher level transitions, and which have already been discussed in section 5.1, are not caught by the Jaynes–Cummings approach. For the resonant case ($\Omega = \Delta_0$), we find that the Jaynes–Cummings method predicts $\omega_{10}$ to be slightly dominating whereas the approach starting from $\mathcal{H}_{QHO}$ results in $\omega_2$ being dominating. The reason for this discrepancy is that due to the counter-rotating terms we have for $\mathcal{H}_{QHO}$ no
symmetric or antisymmetric superposition of the unperturbed eigenstates at $\Omega = \Delta_0$ in contrast to the Jaynes–Cummings model.

To conclude this section, we can say that for an unbiased TLS–HO system the Jaynes–Cummings model gives a good insight into the qualitative behaviour of $P(t)$ both for a slightly detuned and a non-detuned system. However, it under- or overestimates dephasing times for the system. Furthermore, we find taking into account counter-rotating terms in $\hat{H}_{QHO}$ that at $\Omega = \Delta_b$ the dressed eigenstates are not a symmetric or antisymmetric superposition of the uncoupled states. Moreover, the effects of transitions between states of different manifolds are neglected.

7. Conclusions

In conclusion, we discussed the dynamics of a biased and unbiased TLS coupled through a HO to an environmental bath described by an Ohmic spectral density. In particular, we examined the regime of weak damping and moderate coupling between oscillator and TLS. An equivalent description of our system is provided by the spin-boson model with a structured spectral density. In contrast to many other works in this field, our starting point was not the Jaynes–Cummings Hamiltonian, but a more general one given in (1), where no initial RWA has been applied. In section 2.2, we provided with (13) a formal expression for the population difference and showed in section 3.1 how the Hamiltonian of the coupled qubit–HO system can be diagonalized approximately using the Van Vleck perturbation theory. This approach is valid both for the oscillator being in resonance with the qubit ($\Omega = \Delta_b$) and for finite detuning ($|\delta| \neq 0$). In section 3.2, an analytical expression for the non-dissipative dynamics was provided up to second order in the qubit–HO coupling $g$ taking into account the infinite Hilbert space of the system. For low temperatures ($k_BT < \hbar \Omega, \hbar \Delta_b$), we truncated the Hilbert space and found that transition processes between the ground state and the two first excited energy levels of the qubit–HO system dominate the dynamics (section 3.3). In section 4, the influence of the bath was taken into account by solving the Born–Markov master equation for the density matrix of the qubit–HO system. To do this analytically, we considered two variants of the secular approximation: firstly, in section 4.3.1, the FSA, where all fast oscillating terms are neglected, and secondly, in section 4.3.3, the PSA, where attention was paid to the fact that the first two excited energy levels are almost degenerate. Using an ansatz for the long time dynamics in section 4.3.2, we could provide a general expression for the relaxation and dephasing rates of the qubit, showing that the relaxation time can be enhanced by detuning the oscillator into the off-resonant regime. It was found that all three approaches agree quite well with the numerical solution of the master equation. The dynamics of both a biased and an unbiased qubit were intensively studied for zero and finite detuning in section 5. The results agree qualitatively with the numerical findings within the ab initio QUAPI approach [27]. Furthermore, in section 5.1, a good agreement with the results of the WDA performed in [31] for a symmetric spin-boson model was found. Besides, we saw that at resonance ($\Omega = \Delta_b$) the first two excited qubit oscillator states are not a symmetric or antisymmetric superposition of the states $|0e\rangle$ and $|1g\rangle$, as predicted by the Jaynes–Cummings model, and thus could give an explanation for the differently weighted peaks of $\omega_{10}$ and $\omega_{20}$ in the Fourier spectrum of the dynamics. We further could explain the dominance of frequency $\omega_{20}$ in the case of negative detuning ($\Omega < \Delta_b$) and of frequency $\omega_{10}$ for positive detuning, respectively. Moreover, we showed that for large negative detuning $\omega_{20}$ approaches the energy splitting $\Delta_b$ of the qubit, whereas $\omega_{10}$ approximates the
oscillator frequency $\Omega$. This behaviour agrees nicely with spectroscopic experiments performed on a circuit QED architecture [13]. In section 6, we compared our results for an unbiased system to the ones obtained starting with the Jaynes–Cummings model. We visualize the effects of the counter-rotating terms in the Bloch–Siegert shift of the resonance frequency and in contributions of states with larger oscillator number to the TLS dynamics. Apart from this, the Jaynes–Cummings model and our approach agree quite well for the non-dissipative case. Also for the dissipative case at resonance an initial RWA represents a good approximation to our starting Hamiltonian and seems to be favourable as it is analytically exactly diagonalizable. For detuned systems, however, we find discrepancies concerning relaxation and dephasing times and a RWA becomes less appropriate to give precise results. Thus, we think that our approach represents an improvement as it is valid in a wider parameter range avoiding an initial RWA. To our knowledge it provides for the first time analytical results for the dynamics of an unbiased and biased qubit coupled to a structured environment being valid both in the resonant and off-resonant regimes. Furthermore, due to the generality of the qubit–oscillator model, we expect our results to be of interest for a wide range of experimental applications.

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Appendix A. Formula for the dynamics

Here, we show how to derive (13) given in section 2.2. In order to trace out the oscillator degrees of freedom, we transform $\rho_{nm}(t)$ into the basis $\{|jg\}; |je\rangle$ and by using $\rho_{nm} = \rho_{mn}^*$, we find

$$\rho_{jg,jg}(t) = \langle jg | \rho(t) | jg \rangle = \sum_n \langle jg | n \rangle^2 \rho_{nn}(t) + \sum_{n \neq m} \text{Re} \{ \rho_{nm}(t) \} | jg | n \rangle \langle m | jg \rangle,$$

(A.1a)

$$\rho_{je,je}(t) = \langle je | \rho(t) | je \rangle = \sum_n \langle je | n \rangle^2 \rho_{nn}(t) + \sum_{n \neq m} \text{Re} \{ \rho_{nm}(t) \} | je | n \rangle \langle m | je \rangle.$$  

(A.1b)

Performing the trace over the oscillator

$$\rho_{\text{red,gg}}(t) = \langle g | \rho_{\text{red}}(t) | g \rangle = \sum_{j=0}^{\infty} \sum_n \langle jg | n \rangle^2 \rho_{nn}(t) + \sum_{j=0}^{\infty} \sum_{n \neq m} \text{Re} \{ \rho_{nm}(t) \} | jg | n \rangle \langle m | jg \rangle,$$

(A.2a)

$$\rho_{\text{red,ee}}(t) = \langle e | \rho_{\text{red}}(t) | e \rangle = \sum_{j=0}^{\infty} \sum_n \langle je | n \rangle^2 \rho_{nn}(t) + \sum_{j=0}^{\infty} \sum_{n \neq m} \text{Re} \{ \rho_{nm}(t) \} | je | n \rangle \langle m | je \rangle.$$  

(A.2b)

Similarly, we find for the off-diagonal elements of the reduced density matrix

$$\rho_{\text{red,eg}}(t) = \sum_{j=0}^{\infty} \sum_n \langle je | n \rangle \rho_{nn}(t) | n | jg \rangle$$

$$+ \frac{1}{2} \sum_{j=0}^{\infty} \sum_{n \neq m} \left[ \langle je | n \rangle \rho_{nm}(t) | m | jg \rangle + \langle je | m \rangle \rho_{nm}^*(t) | jg | n \rangle \right].$$

(A.3a)
\[ \rho_{\text{red;ge}}(t) = \sum_{j=0}^{\infty} \sum_{n} \langle jg|n \rangle \rho_{nn}(t) \langle n|je \rangle \]
\[ + \frac{1}{2} \sum_{j=0}^{\infty} \sum_{n,m, n \neq m} \left[ \langle jg|n \rangle \rho_{mn}(t) \langle m|je \rangle + \langle jg|m \rangle \rho_{nm}^*(t) \langle je|n \rangle \right]. \quad (A.3b) \]

Using (5) and (6) in (11) we can express \( P(t) \) in the energy basis, yielding
\[ P(t) = \cos \Theta [\rho_{\text{red;gg}}(t) - \rho_{\text{red;ee}}(t)] + \sin \Theta [\rho_{\text{red;ge}}(t) + \rho_{\text{red;eg}}(t)] \]
\[ = \cos(\Theta) \left( \sum_{j=0}^{\infty} \sum_{n} \left[ \langle jg|n \rangle^2 - \langle je|n \rangle^2 \right] \rho_{nn}(t) \right. \]
\[ + \sum_{j=0}^{\infty} \sum_{n,m, n \neq m} \left[ \langle jg|n \rangle \langle m|jg \rangle - \langle jg|n \rangle \langle m|jg \rangle \right] \text{Re} \{ \rho_{nm}(t) \} \bigg) \]
\[ + \sin(\Theta) \left( 2 \sum_{j=0}^{\infty} \sum_{n} \langle je|n \rangle \rho_{nn}(t) \langle n|jg \rangle \right. \]
\[ + \sum_{j=0}^{\infty} \sum_{n,m, n \neq m} \left[ \langle je|n \rangle \langle m|jg \rangle + \langle je|m \rangle \langle jg|n \rangle \right] \text{Re} \{ \rho_{nm}(t) \} \right). \quad (A.4) \]

With (28) we can write
\[ P(t) = \sum_{n} p_{nn}(t) + \sum_{n,m, n \neq m} p_{nm}(t) \cos \omega_{nm} t, \quad (A.5) \]
where
\[ p_{nn}(t) = \sum_{j} \left\{ \cos \Theta \left[ \langle jg|n \rangle^2 - \langle je|n \rangle^2 \right] + 2 \sin \Theta \langle jg|n \rangle \langle je|n \rangle \right\} \rho_{nn}(t). \quad (A.6a) \]
\[ p_{nm}(t) = 2 \sum_{j} \left\{ \cos \Theta \left[ \langle jg|n \rangle \langle m|jg \rangle - \langle je|n \rangle \langle m|je \rangle \right] \right. \]
\[ + \sin \Theta \left[ \langle je|n \rangle \langle m|jg \rangle + \langle je|m \rangle \langle jg|n \rangle \right] \text{Re} \{ \rho_{nm}(t) \} \right\}. \quad (A.6b) \]

**Appendix B. The Van Vleck perturbation theory**

Let us consider the Hamiltonian
\[ \mathcal{H} = \mathcal{H}_0 + V \quad (B.1) \]
consisting of the free Hamiltonian \( \mathcal{H}_0 \) and a small perturbation \( V \sim g \), which is proportional to the coupling constant \( g \). Additionally we assume that the energy levels \( E_{j,\alpha} \) of \( \mathcal{H}_0 \) are grouped into manifolds with \( \alpha \) being the index of the manifold and \( i \) is used to distinguish between
different energy levels within the same manifold. The energy levels \( E_{j,\alpha} \) are eigenenergies of \( \mathcal{H}_0 \):

\[
\mathcal{H}_0 | j, \alpha \rangle = E_{j,\alpha} | j, \alpha \rangle.
\]

Through the perturbation \( V \) different manifolds are coupled together. As long as the coupling \( g \) is small, namely that \(|\langle j, \alpha | V | j, \beta \rangle| \ll |E_{j,\alpha} - E_{j,\beta}| \) for \( \alpha \neq \beta \), also the energy levels of the total Hamiltonian \( \mathcal{H} \) are clustered into manifolds. Using the transformation \( \mathcal{H}_{\text{eff}} = e^{iS} \mathcal{H} e^{-iS} \), we construct an effective Hamiltonian \( \mathcal{H}_{\text{eff}} \), which acts only within the individual manifolds; i.e. \( \langle j, \alpha | \mathcal{H}_{\text{eff}} | j, \beta \rangle = 0 \) for \( \alpha \neq \beta \), and has the same eigenvalues as \( \mathcal{H} \) within the manifolds. We expand \( S \) and \( \mathcal{H}_{\text{eff}} \) in terms of the small parameter \( g \) up to second order:

\[
S = S^{(1)} + S^{(2)} + O(g^3) \quad \text{and} \quad \mathcal{H}_{\text{eff}} = \mathcal{H}_{\text{eff}}^{(0)} + \mathcal{H}_{\text{eff}}^{(1)} + \mathcal{H}_{\text{eff}}^{(2)} + O(g^3).
\]

For calculating \( S^{(1/2)} \) and \( \mathcal{H}_{\text{eff}}^{(1/2)} \), we use that \( \langle j, \alpha | \mathcal{H}_{\text{eff}}^{(1/2)} | j, \beta \rangle = 0 \) for \( \alpha \neq \beta \) and furthermore choose that \( S \) has no matrix elements within a manifold, namely \( \langle j, \alpha | S^{(1/2)} | j, \alpha \rangle = 0 \). Now, one can iteratively calculate \( S \) and \( \mathcal{H}_{\text{eff}} \) order by order. For details see [41]. Here, we give only the results. For the transformation one has

\[
\langle j, \alpha | iS^{(1)} | j, \beta \rangle = \frac{\langle j, \alpha | V | j, \beta \rangle}{E_{j,\beta} - E_{j,\alpha}}, \quad \text{for} \quad \alpha \neq \beta,
\]

and

\[
\langle j, \alpha | iS^{(2)} | j, \beta \rangle = \frac{1}{2} \sum_{k, \gamma \neq \alpha, \beta} \frac{\langle j, \alpha | V | k, \gamma \rangle \langle k, \gamma | V | j, \beta \rangle}{E_{j,\beta} - E_{j,\alpha}} \left[ \frac{1}{E_{k,\gamma} - E_{j,\alpha}} + \frac{1}{E_{k,\gamma} - E_{j,\beta}} \right] \\
+ \sum_{k} \frac{1}{E_{j,\beta} - E_{j,\alpha}} \frac{\langle j, \alpha | V | k, \beta \rangle \langle k, \beta | V | j, \beta \rangle}{E_{k,\beta} - E_{j,\alpha}} \\
+ \sum_{k} \frac{1}{E_{j,\beta} - E_{j,\alpha}} \frac{\langle j, \alpha | V | k, \alpha \rangle \langle k, \alpha | V | j, \beta \rangle}{E_{k,\alpha} - E_{j,\beta}}, \quad \text{for} \quad \alpha \neq \beta.
\]

The effective Hamiltonian is up to second order

\[
\langle i, \alpha | \mathcal{H}_{\text{eff}} | j, \alpha \rangle = E_{j,\alpha} \delta_{ij} + \langle i, \alpha | V | j, \alpha \rangle \\
+ \frac{1}{2} \sum_{k, \gamma \neq \alpha} \langle i, \alpha | V | k, \gamma \rangle \langle k, \gamma | V | j, \alpha \rangle \left[ \frac{1}{E_{i,\alpha} - E_{k,\gamma}} + \frac{1}{E_{i,\alpha} - E_{k,\gamma}} \right] + O(g^3).
\]

In the case of the Hamiltonian \( \mathcal{H}_{\text{QHO}} \), the first-order matrix elements are

\[
iS_{E_{j-1}}^{(1)} = -\sqrt{j} \frac{\varepsilon}{\Delta_b \Omega} g,
\]

\[
iS_{E_{j+1}}^{(1)} = -\sqrt{j+1} \frac{\varepsilon}{\Delta_b \Omega} g,
\]

\[
iS_{E_{j+1}}^{(1)} = \sqrt{j+1} \frac{\Delta_0}{\Delta_b (\Delta_b + \Omega)} g,
\]

and for the second-order contributions

\[
iS_{E_{j+2}}^{(2)} = 2\sqrt{(j+1)(j+2)} \frac{\varepsilon \Delta_0}{\Delta_b^2 (2\Omega - \Delta_b)} g^2.
\]
Here, we give the matrix elements specified in section 4.2.

4.2 Matrix Elements

Here, we give the matrix elements \(X_{nm}\) specified in section 4.2.

\[
X_{2j+1,2j+1} = -2L_0 \cos \alpha_j + \sqrt{j + 1} L_{q,\text{osc}}^+ \sin \alpha_j,
\]

\[
X_{2j+1,2j+2} = 2L_0 \sin \alpha_j + \sqrt{j + 1} L_{q,\text{osc}}^- \cos \alpha_j,
\]

\[
X_{2j+1,2j+3} = L_q \cos(\alpha_j/2) \sin(\alpha_{j+1}/2) + \sqrt{j + 2} (1 + L_{\text{osc}}) \cos(\alpha_j/2) \cos(\alpha_{j+1}/2)
\]

\[
+ \sqrt{j + 1} (1 - L_{\text{osc}}) \sin(\alpha_j/2) \sin(\alpha_{j+1}/2),
\]

\[
X_{2j+1,2j+4} = L_q \cos(\alpha_j/2) \sin(\alpha_{j+1}/2) - \sqrt{j + 2} (1 + L_{\text{osc}}) \cos(\alpha_j/2) \sin(\alpha_{j+1}/2)
\]

\[
+ \sqrt{j + 1} (1 - L_{\text{osc}}) \sin(\alpha_j/2) \cos(\alpha_{j+1}/2),
\]

\[
X_{2j+1,2j+5} = \sqrt{j + 2} L_{q,\text{osc}}^+ \cos(\alpha_j/2) \sin(\alpha_{j+1}/2),
\]

\[
X_{2j+1,2j+6} = \sqrt{j + 2} L_{q,\text{osc}}^+ \cos(\alpha_j/2) \cos(\alpha_{j+1}/2),
\]

\[
X_{2j+2,2j+2} = 2L_0 \cos \alpha_j - \sqrt{j + 1} L_{q,\text{osc}}^- \sin \alpha_j,
\]

\[
X_{2j+2,2j+3} = -L_q \sin(\alpha_j/2) \sin(\alpha_{j+1}/2) - \sqrt{j + 2} (1 + L_{\text{osc}}) \sin(\alpha_j/2) \cos(\alpha_{j+1}/2)
\]

\[
+ \sqrt{j + 1} (1 - L_{\text{osc}}) \cos(\alpha_j/2) \sin(\alpha_{j+1}/2),
\]

\[
X_{2j+2,2j+4} = -L_q \sin(\alpha_j/2) \cos(\alpha_{j+1}/2) + \sqrt{j + 2} (1 + L_{\text{osc}}) \sin(\alpha_j/2) \sin(\alpha_{j+1}/2)
\]

\[
+ \sqrt{j + 1} (1 - L_{\text{osc}}) \cos(\alpha_j/2) \cos(\alpha_{j+1}/2),
\]

\[
X_{2j+2,2j+5} = -\sqrt{j + 2} L_{q,\text{osc}}^+ \sin(\alpha_j/2) \sin(\alpha_{j+1}/2),
\]

\[
X_{2j+2,2j+6} = -\sqrt{j + 2} L_{q,\text{osc}}^+ \sin(\alpha_j/2) \cos(\alpha_{j+1}/2).
\]
Matrix elements including the ground state are given separately because of the special shape of |0⟩:

\[ X_{0,0} = -2L_0, \]
\[ X_{0,1} = \sin(\alpha_0/2)L_q + \cos(\alpha_0/2)(1 + L_{\text{osc}}), \]
\[ X_{0,2} = \cos(\alpha_0/2)L_q - \sin(\alpha_0/2)(1 + L_{\text{osc}}), \]
\[ X_{0,3} = \sin(\alpha_1/2)L_{\text{osc}q}, \]
\[ X_{0,4} = \cos(\alpha_1/2)L_{q\text{osc}}. \]

All other matrix elements are zero.

Appendix D. Rate coefficients for the off-diagonal density matrix elements

Here, we give the rate coefficients of the master equation for the reduced density matrix elements. They are:

\[ \mathcal{L}_{01,01} = \frac{4\kappa}{\hbar\beta}L_0^2(2 \cos \alpha_0 - \cos^2 \alpha_0 - 1) - \frac{1}{2} \mathcal{L}_{00,11}, \]  
\[ \mathcal{L}_{02,02} = \frac{4\kappa}{\hbar\beta}L_0^2(-2 \cos \alpha_0 - \cos^2 \alpha_0 - 1) - \frac{1}{2} \mathcal{L}_{00,22}, \]  
\[ \mathcal{L}_{03,03} = \frac{4\kappa}{\hbar\beta}L_0^2(2 \cos \alpha_1 - \cos^2 \alpha_1 - 1) - \frac{1}{2} \mathcal{L}_{11,33} \]  
\[ - \frac{1}{2} \mathcal{L}_{22,33}, \]  
\[ \mathcal{L}_{04,04} = \frac{4\kappa}{\hbar\beta}L_0^2(-2 \cos \alpha_1 - \cos^2 \alpha_1 - 1) - \frac{1}{2} \mathcal{L}_{11,44} \]  
\[ - \frac{1}{2} \mathcal{L}_{22,44}, \]  
\[ \mathcal{L}_{12,12} = -\frac{16\kappa}{\hbar\beta}L_0^2 \cos^2 \alpha_0 - \frac{1}{2} \mathcal{L}_{00,11} \]  
\[ - \frac{1}{2} \mathcal{L}_{00,22}, \]  
\[ \mathcal{L}_{13,13} = -\frac{4\kappa}{\hbar\beta}L_0^2(\cos \alpha_0 - \cos \alpha_1)^2 \]  
\[ - \frac{1}{2} \mathcal{L}_{00,11} \]  
\[ - \frac{1}{2} \mathcal{L}_{11,33} \]  
\[ - \frac{1}{2} \mathcal{L}_{22,33}, \]  
\[ \mathcal{L}_{14,14} = -\frac{4\kappa}{\hbar\beta}L_0^2(\cos \alpha_0 + \cos \alpha_1)^2 \]  
\[ - \frac{1}{2} \mathcal{L}_{00,11} \]  
\[ - \frac{1}{2} \mathcal{L}_{11,44} \]  
\[ - \frac{1}{2} \mathcal{L}_{22,44}, \]  
\[ \mathcal{L}_{23,23} = -\frac{4\kappa}{\hbar\beta}L_0^2(\cos \alpha_0 + \cos \alpha_1)^2 \]  
\[ - \frac{1}{2} \mathcal{L}_{00,22} \]  
\[ - \frac{1}{2} \mathcal{L}_{11,33} \]  
\[ - \frac{1}{2} \mathcal{L}_{22,33}, \]  
\[ \mathcal{L}_{24,24} = -\frac{4\kappa}{\hbar\beta}L_0^2(\cos \alpha_0 - \cos \alpha_1)^2 \]  
\[ - \frac{1}{2} \mathcal{L}_{00,22} \]  
\[ - \frac{1}{2} \mathcal{L}_{11,44} \]  
\[ - \frac{1}{2} \mathcal{L}_{22,44}, \]  
\[ \mathcal{L}_{12,12} = -\frac{16\kappa}{\hbar\beta}L_0^2 \cos^2 \alpha_1 \]  
\[ - \frac{1}{2} \mathcal{L}_{11,33} \]  
\[ - \frac{1}{2} \mathcal{L}_{22,33} \]  
\[ - \frac{1}{2} \mathcal{L}_{11,44} \]  
\[ - \frac{1}{2} \mathcal{L}_{22,44}, \]  
\[ \mathcal{L}_{01,02} = \frac{4\kappa}{\hbar\beta}(X_{00}X_{12} - X_{12}X_{00}) \]  
\[ - G(\omega_0)N_{02}X_{01}X_{02} \]  
\[ - G(\omega_1)N_{12}X_{11}X_{12} \]  
\[ - G(\omega_2)N_{32}X_{13}X_{23} \]  
\[ - G(\omega_4)N_{42}X_{14}X_{24}, \]  
\[ (D.11) \]
The solutions of the FSA master equation (51) for the diagonal elements reads:

\[
\sigma_{00}(t) = \sigma_{00}^0 + \sigma_{11}^0 + \sigma_{22}^0 + \sigma_{33}^0 + \sigma_{44}^0
\]

\[
- e^{-\pi \mathcal{L}_{00,11} t} \left( \sigma_{11}^0 + \sigma_{22}^0 \frac{\mathcal{L}_{11,33}}{-\mathcal{L}_{00,11} + \mathcal{L}_{11,33} + \mathcal{L}_{22,33}} + \sigma_{44}^0 \frac{\mathcal{L}_{11,44}}{-\mathcal{L}_{00,11} + \mathcal{L}_{11,44} + \mathcal{L}_{22,44}} \right)
\]

\[
- e^{-\pi \mathcal{L}_{00,22} t} \left( \sigma_{22}^0 + \sigma_{33}^0 \frac{\mathcal{L}_{22,33}}{-\mathcal{L}_{00,22} + \mathcal{L}_{11,33} + \mathcal{L}_{22,33}} + \sigma_{44}^0 \frac{\mathcal{L}_{22,44}}{-\mathcal{L}_{00,22} + \mathcal{L}_{11,44} + \mathcal{L}_{22,44}} \right)
\]

\[
+ e^{-\pi (\mathcal{L}_{11,33} + \mathcal{L}_{22,33}) t} \sigma_{33}^0 \left( \frac{\mathcal{L}_{00,22} - \mathcal{L}_{11,33}}{-\mathcal{L}_{00,22} + \mathcal{L}_{11,33} + \mathcal{L}_{22,33}} + \frac{\mathcal{L}_{11,33}}{-\mathcal{L}_{00,11} + \mathcal{L}_{11,33} + \mathcal{L}_{22,33}} \right)
\]

\[
+ e^{-\pi (\mathcal{L}_{11,44} + \mathcal{L}_{22,44}) t} \sigma_{44}^0 \left( \frac{\mathcal{L}_{00,22} - \mathcal{L}_{11,44}}{-\mathcal{L}_{00,22} + \mathcal{L}_{11,44} + \mathcal{L}_{22,44}} + \frac{\mathcal{L}_{11,44}}{-\mathcal{L}_{00,11} + \mathcal{L}_{11,44} + \mathcal{L}_{22,44}} \right),
\]

\[
(\text{E.1})
\]

\[
\sigma_{11}(t) = - e^{-\pi \mathcal{L}_{00,11} t} \sigma_{11}^0
\]

\[
- e^{-\pi (\mathcal{L}_{00,11} + \mathcal{L}_{11,33} + \mathcal{L}_{22,33}) t} \sigma_{33}^0 \frac{\mathcal{L}_{11,33}}{-\mathcal{L}_{00,11} + \mathcal{L}_{11,33} + \mathcal{L}_{22,33}}
\]

\[
- e^{-\pi (\mathcal{L}_{00,11} + \mathcal{L}_{11,44} + \mathcal{L}_{22,44}) t} \sigma_{44}^0 \frac{\mathcal{L}_{11,44}}{-\mathcal{L}_{00,11} + \mathcal{L}_{11,44} + \mathcal{L}_{22,44}}.
\]

\[
(\text{E.2})
\]

**Appendix E. Diagonal reduced density matrix elements**

The solutions of the FSA master equation (51) for the diagonal elements reads:
\[ \sigma_{22}(t) = -e^{-\pi \mathcal{L}_{00,22}} \sigma_{22}^0 - e^{-\pi (\mathcal{L}_{00,22} + \mathcal{L}_{11,33} + \mathcal{L}_{22,33})} \sigma_{33}^0 \mathcal{L}_{22,33} - e^{-\pi (\mathcal{L}_{00,22} + \mathcal{L}_{11,44} + \mathcal{L}_{22,44})} \sigma_{44}^0 \mathcal{L}_{22,44} - e^{-\pi (\mathcal{L}_{00,22} + \mathcal{L}_{11,33} + \mathcal{L}_{22,33})} \sigma_{33}^0 - e^{-\pi (\mathcal{L}_{00,22} + \mathcal{L}_{11,44} + \mathcal{L}_{22,44})} \sigma_{44}^0 \mathcal{L}_{22,44} , \]

(E.3)

\[ \sigma_{33}(t) = e^{-\pi (\mathcal{L}_{11,33} + \mathcal{L}_{22,33})} \sigma_{33}^0 , \quad \sigma_{44}(t) = e^{-\pi (\mathcal{L}_{11,44} + \mathcal{L}_{22,44})} \sigma_{44}^0 . \]

(E.4)

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