Dynamics of the dissipative four-state system

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Abstract

Abstract goes here

Dedication

To mum and dad

Declaration

I declare that..

Acknowledgements

I want to thank...

Contents

1 Introduction

This thesis will discuss the dynamics of a quantum mechanical four-state system, which is coupled to a photonic mode in an optical cavity.

2 Theoretical foundations

The bath correlation function in this case takes the form

$$Q(t) = S(t) + iR(t) = \int_0^\infty \mathsf{d}\omega \frac{J(\omega)}{\omega^2} \coth\frac{\hbar\omega\beta}{2} \Big[(1-\cos\omega t) + i\sin\omega t\Big] \psi\mathcal{E}. \tag{2.1}$$

3 The doublet-doublet system

In this chapter, we will consider the system of a single particle with mass $\mathcal{M}$, position operator $\mathbf{q}$ and momentum operator $\mathbf{p}$. The particle is placed in a double-well potential, giving the Hamiltionian

$$\mathbf{H}_{\mathrm{DW}} = \frac{\mathbf{p}^2}{2\mathcal{M}} + \frac{\mathcal{M}^2\omega_0^4}{64\Delta U}\mathbf{q}^4 - \frac{\mathcal{M}\omega_0^2}{4}\mathbf{q}^2 - \mathbf{q}\epsilon. \tag{3.1}$$

Here, ΔU is the barrier height, ω_0 is the classical oscillation frequency and ϵ is the bias factor of the double-well potential. In addition, we introduce a single cavity mode, which couples linearly to the doublet-doublet system and is described by

$$\mathbf{H}_{C,\mathrm{int}} = \Omega\mathbf{a}^\dagger\mathbf{a} + g\mathbf{q}\left(\mathbf{a} + \mathbf{a}^\dagger\right). \tag{3.2}$$

Next, the cavity mode is coupled to a bath consisting of simple harmonic oscillators. For now, we will neglect the direct coupling of the DW-system to a bath:

$$\mathbf{H}_{B,\mathrm{int}} = \left(\mathbf{a} + \mathbf{a}^\dagger\right)\sum_k \nu_k\left(\mathbf{b}_k + \mathbf{b}_k^\dagger\right) + \sum_k \omega_k\mathbf{b}_k^\dagger\mathbf{b}_k. \tag{3.3}$$

For the cavity mode, we choose Ohmic damping. In the continuous limit, this means the spectral density is given by

$$J_{\mathrm{Ohm}}\left(\omega\right) = \sum_k \nu_k^2\delta\left(\omega - \omega_k\right) = \kappa\omega e^{-\omega/\omega_c}, \tag{3.4}$$

where κ is the cavity damping constant and ω_c is the cut-off frequency.
According to Garg, Onuchic and Ambegaokar, this model can be mapped to a double-well coupling to a bath with a peaked spectral density with the coupling term

$$\mathbf{H}_{B,\mathrm{DW}} = \mathbf{q}\sum_k \lambda_k\left(\tilde{\mathbf{a}}_k + \tilde{\mathbf{a}}_k^\dagger\right) + \sum_k \tilde{\omega}_k\tilde{\mathbf{a}}_k^\dagger\tilde{\mathbf{a}}_k. \tag{3.5}$$

and the effective bath spectral density

$$J\left(\omega\right) = \sum_k \lambda_k^2\delta\left(\omega - \tilde{\omega}_k\right) = \frac{2\alpha\omega\Omega^4}{\left(\Omega^2 - \omega^2\right)^2 + \left(2\pi\kappa\omega\Omega\right)^2}, \tag{3.6}$$

where $\alpha = 8\kappa g^2/\Omega^2$ is the effective low-frequency damping constant. In the low-frequence limit, i.e. $\omega \to 0$, the effective bath spectral density reduces to $J\left(\omega\right) \to 2\alpha\omega$.

3.1 The DW-system in the DVR-basis

3.2 Calculation of the Rate Matrix Elements

The Markov-approximated rate matrix elements read, to lowest order,

$$\Gamma_{\mu\nu}^{(2)} = \frac{\Delta_{\mu\nu}^2}{2}\int_0^\infty \mathrm{d}\tau e^{-\left(q_\mu - q_\nu\right)^2 S(\tau)}\cos\left[\left(E_\mu - E_\nu\right)\tau + \left(q_\mu - q_\nu\right)^2 R\left(\tau\right)\right], \tag{3.7}$$

where $S(\tau)$ and $R(\tau)$ are the real and complex parts of the twice integrated bath autocorrelation function reading

$$Q(\tau) = S(\tau) + \mathrm{i}R(\tau) = \frac{1}{\pi}\int_0^\infty \mathrm{d}\omega \frac{J(\omega)}{\omega^2} \coth\frac{\hbar\omega\beta}{2}\Big[(1-\cos\omega\tau) + \mathrm{i}\sin\omega\tau\Big]. \tag{3.8}$$

Inserting the bath spectral density (3.6) and defining the width of the peaked bath spectral density, $\Gamma = 2\pi\kappa\Omega$, one obtains the integral

$$S(\tau) + \mathrm{i}R(\tau) = \frac{2\alpha}{\pi}\int_0^\infty \mathrm{d}\omega \frac{1}{\omega}\frac{\Omega^4}{(\Omega^2-\omega^2)^2 + (\Gamma\omega)^2} \coth\frac{\hbar\omega\beta}{2}\Big[(1-\cos\omega\tau) + \mathrm{i}\sin\omega\tau\Big]. \tag{3.9}$$

We will now evaluate the real and complex part of the integral seperately. The real part reads

$$S(\tau) = \frac{2\alpha}{\pi}\int_0^\infty \mathrm{d}\omega \frac{1}{\omega}\frac{\Omega^4}{(\Omega^2-\omega^2)^2 + (\Gamma\omega)^2} \coth\frac{\hbar\omega\beta}{2}(1-\cos\omega\tau). \tag{3.10}$$

Using the symmetry of the integrand with respect to $\omega \to -\omega$, one can rewrite the integral as

$$S(\tau) = \frac{\alpha}{\pi}\int_{-\infty}^\infty \mathrm{d}\omega \frac{1}{\omega}\frac{\Omega^4}{(\Omega^2-\omega^2)^2 + (\Gamma\omega)^2} \coth\frac{\hbar\omega\beta}{2}\left(1-e^{\mathrm{i}\omega\tau}\right). \tag{3.11}$$

This expression is best solved using the residue theorem. For this, we need to determine the poles of the integrand. The first factor only as a pole of order 1 at $\omega_0 = 0$. To find the poles of the second factor, one has to solve the equation

$$\left(\Omega^2-\omega^2\right)^2 + (\Gamma\omega)^2 = 0. \tag{3.12}$$

Solving this equation is easily performed by simple algebra and yields the following simple poles:

$$\omega_{1,2,3,4} = \pm\frac{\mathrm{i}\Gamma}{2} \pm \sqrt{\frac{\Gamma^2}{4} + \Omega^2} = \pm\bar{\Omega} \pm \frac{\mathrm{i}\Gamma}{2}, \tag{3.13}$$

after defining $\bar{\Omega} = \sqrt{\Gamma^2/4 + \Omega^2}$. Turning to the third factor, we recall the fact that the hyperbolic cotangent has simple poles at $x = \mathrm{i}k\pi,\ k \in \mathbb{Z}$. After some calculation, the poles of $\coth(\hbar\omega\beta/2)$ are resolved to be

$$\omega = \mathrm{i}\frac{2\pi k}{\hbar\beta} = \mathrm{i}\nu_k,\ \ k \in \mathbb{Z}, \tag{3.14}$$

where the ν_k are the so-called bosonic Matsubara frequencies. As the fourth factor does not possess any poles, we have now identified every pole exhibited by the integrand. Next, we have to choose a suitable integration contour. Here, we choose the half annulus lieing in the upper complex half-plane with outer radius R and inner radius r. Using this contour, the real part of the bath autocorrelation function is given by

$$\int_{-\infty}^\infty \mathrm{d}\omega F(\omega) = 2\pi\mathrm{i}\sum_k \mathrm{Res}(F,\omega_k) - \lim_{R\to\infty}\int_{\mathcal{C}_1}\mathrm{d}\omega F(\omega) - \lim_{r\to 0}\int_{\mathcal{C}_2}\mathrm{d}\omega F(\omega), \tag{3.15}$$

where $\mathcal{C}_1$ is the outer half-circle and $\mathcal{C}_2$ is the inner half-circle of the contour and the ω_k denote the poles of the integrand. In the limit $R \to \infty$ and $r \to 0$, we will pick-up all of the poles which lie in the upper complex half-plane, namely ω_1, ω_2 and $\mathrm{i}\nu_n$ for $n > 0$. Performing the calculation of the residues and limits with some care results in

$$S(\tau) = X\tau + L\Big(e^{-(\Gamma/2)\tau}\cos\bar{\Omega}\tau - 1\Big) + Ze^{-(\Gamma/2)\tau}\sin\bar{\Omega}\tau + S_{\mathrm{Mats}}(\tau), \tag{3.16}$$

with the prefactors being

$$L = \frac{\alpha}{\Gamma\bar{\Omega}}\frac{1}{\cosh(\hbar\beta\bar{\Omega}) - \cos(\hbar\beta\Gamma/2)}\left[\left(\frac{\Gamma^2}{4} - \bar{\Omega}^2\right)\sinh(\hbar\beta\bar{\Omega}) + \Gamma\bar{\Omega}\sin(\hbar\beta\Gamma/2)\right], \tag{3.17}$$

$$Z = \frac{\alpha}{\Gamma\bar{\Omega}} \frac{1}{\cosh(\hbar\beta\bar{\Omega}) - \cos(\hbar\beta\Gamma/2)} \left[-\Gamma\bar{\Omega}\sinh(\hbar\beta\bar{\Omega}) + \left(\frac{\Gamma^2}{4} - \bar{\Omega}^2 \right) \sin(\hbar\beta\Gamma/2) \right], \tag{3.18}$$

and $X = 2\alpha/(\hbar\beta)$. The last term $S_{\mathrm{Mats}}(\tau)$ reads

$$S_{\mathrm{Mats}}(\tau) = -\frac{4\alpha\Omega^4}{\hbar\beta} \sum_{n=1}^{\infty} \frac{1}{(\Omega^2 + \nu_n^2)^2 - \Gamma^2\nu_n^2} \left[\frac{e^{-\nu_n\tau} - 1}{\nu_n} \right]. \tag{3.19}$$

Choosing the same contour for the integration of the imaginary part of (3.6),

$$R(\tau) = \frac{2\alpha}{\pi} \int_0^\infty \mathrm{d}\omega \frac{1}{\omega} \frac{\Omega^4}{\left(\Omega^2 - \omega^2\right)^2 + (\Gamma\omega)^2} \sin\omega\tau \tag{3.20}$$

$$= \frac{\alpha}{\pi} \int_{-\infty}^\infty \mathrm{d}\omega \frac{1}{\omega} \frac{\Omega^4}{\left(\Omega^2 - \omega^2\right)^2 + (\Gamma\omega)^2} e^{\mathrm{i}\omega\tau}, \tag{3.21}$$

the imaginary part can be analogously computed to be

$$R(\tau) = \alpha - \alpha e^{-(\Gamma/2)\tau} \left(N \sin\bar{\Omega}\tau + \cos\bar{\Omega}\tau \right), \tag{3.22}$$

where $N = (\Gamma^2/4 - \bar{\Omega}^2)/(\Gamma\bar{\Omega})$. In order to obtain an analytical expression for the rate matrix elements, we will now make the assumption that the bath spectral density is sharply peaked, which means that $\kappa = \Gamma/(2\pi\Omega) \ll 1$. This allows us to expand the bath correlation function $Q(\tau)$ to the first-order in κ. After performing the expansion, we obtain

$$S(\tau) = Y(\cos\Omega\tau - 1) + A\tau\cos\Omega\tau + B\tau\sin\Omega\tau + \mathcal{O}\left[\kappa^2\right], \tag{3.23}$$

$$R(\tau) = W\sin\Omega\tau + V(1 - \cos\Omega\tau - \frac{\Omega}{2}\tau\sin\Omega\tau) + \mathcal{O}\left[\kappa^2\right], \tag{3.24}$$

with the temperature dependent coefficients

$$Y = -\frac{4g^2}{\Omega^2}\coth\frac{\hbar\beta\Omega}{2}, \quad W = \frac{4g^2}{\Omega^2} \tag{3.25}$$

$$A = \frac{4\Gamma g^2}{2\Omega^2}\coth\frac{\hbar\beta\Omega}{2}, \quad B = \frac{8\Gamma g^2}{\Omega^2\hbar\beta} \tag{3.26}$$

$$C = -\frac{2\Gamma g^2}{\Omega^3}\frac{\hbar\beta\Omega + 2\sinh\hbar\beta\Omega}{\cosh\hbar\beta\Omega - 1}, \quad V = \frac{4\Gamma g^2}{\Omega^3}. \tag{3.27}$$

We now turn to the computation of the rate matrix elements. Inserting the real and imaginary parts of the bath correlation function into (3.7), we obtain

$$\begin{aligned} \Gamma_{\mu\nu}^{(2)} = \frac{\Delta_{\mu\nu}^2}{2} \int_0^\infty \mathrm{d}\tau \exp\Big\{ -q_{\mu\nu}^2 Y(\cos\Omega\tau - 1) - q_{\mu\nu}^2 A\tau\cos\Omega\tau - q_{\mu\nu}^2 B\tau\cos\Omega\tau \Big\} \\ \times\cos\Big\{ E_{\mu\nu}\tau + q_{\mu\nu}^2 W\sin\Omega\tau + V\Big(1 - \cos\Omega\tau - \frac{\Omega}{2}\tau\sin\Omega\tau\Big)\Big\}, \end{aligned} \tag{3.28}$$

where we have introduced for clarity $q_{\mu\nu} = q_\mu - q_\nu$ and $E_{\mu\nu} = E_\mu - E_\nu$. After using Euler's formula for the cosine and some rearrangement, we arrive at

$$\Gamma_{\mu\nu}^{(2)} = \frac{\Delta_{\mu\nu}^2}{4} e^{\bar{Y} + \mathrm{i}\bar{V}} \int_0^\infty \mathrm{d}\tau e^{-\bar{B}\tau - \bar{A}\tau\cos\omega\tau} e^{\mathrm{i}E_{\mu\nu}\tau - \mathrm{i}\bar{V}\frac{\Omega}{2}\tau\sin\omega\tau} e^{(-\bar{Y} - \mathrm{i}\bar{V})\cos\omega\tau} e^{(-\bar{C} + \mathrm{i}\bar{W})\sin\omega\tau} + \mathrm{c.c} \tag{3.29}$$

after having absorbed the $q_{\mu\nu}^2$ into the barred time-independent factors and denoting the complex conjugate of the first summand as c.c. We notice that the integral converges if the condition $\bar{B} > \bar{A}$ is fulfilled, which imposes

$$\frac{4}{\hbar\beta\Omega} > \coth\frac{\hbar\beta\Omega}{2}. \tag{3.30}$$

When this requirement holds, we can make further approximations. First, we linearize

$$e^{-\bar{A}\tau\cos\omega\tau} \approx 1 - \bar{A}\tau\cos\omega\tau \tag{3.31}$$

$$e^{-\mathrm{i}\bar{V}\frac{\Omega}{2}\tau\sin\omega\tau} \approx 1 - \mathrm{i}\bar{V}\frac{\Omega}{2}\tau\sin\omega\tau. \tag{3.32}$$

Further, we estimate the product of these linearized terms as

$$\Big(1 - \bar{A}\tau\cos\omega\tau\Big)\Big(1 - \mathrm{i}\bar{V}\frac{\Omega}{2}\tau\sin\omega\tau\Big) \approx 1 - \Big(\frac{\bar{A}}{2} + \frac{\bar{V}\Omega}{4}\Big)\tau e^{\mathrm{i}\Omega\tau} - \Big(\frac{\bar{A}}{2} - \frac{\bar{V}\Omega}{4}\Big)\tau e^{-\mathrm{i}\Omega\tau}. \tag{3.33}$$

Employing the Jacobi-Anger expansions

$$e^{\mathrm{i}z\cos\theta} = \sum_{n=-\infty}^{\infty} \mathrm{i}^n J_n(z) e^{\mathrm{i}n\theta} \tag{3.34}$$

and respectively

$$e^{\mathrm{i}z\sin\theta} = \sum_{n=-\infty}^{\infty} J_n(z) e^{\mathrm{i}n\theta}, \tag{3.35}$$

with $J_n(z)$ being the n-th Bessel function of the first kind, we can rewrite the factors containing trigonometric functions in the exponential as

$$e^{(-\bar{Y}-\mathrm{i}\bar{V})\cos\omega\tau} e^{(-\bar{C}+\mathrm{i}\bar{W})\sin\omega\tau} = \sum_{m,n=-\infty}^{\infty} \mathrm{i}^m J_m(-\bar{V}+\mathrm{i}\bar{Y}) J_n(\bar{W}+\mathrm{i}\bar{C}) e^{\mathrm{i}(m+n)\Omega\tau}. \tag{3.36}$$

Collecting all the recastings and inserting them into (3.29) we arrive at the final form

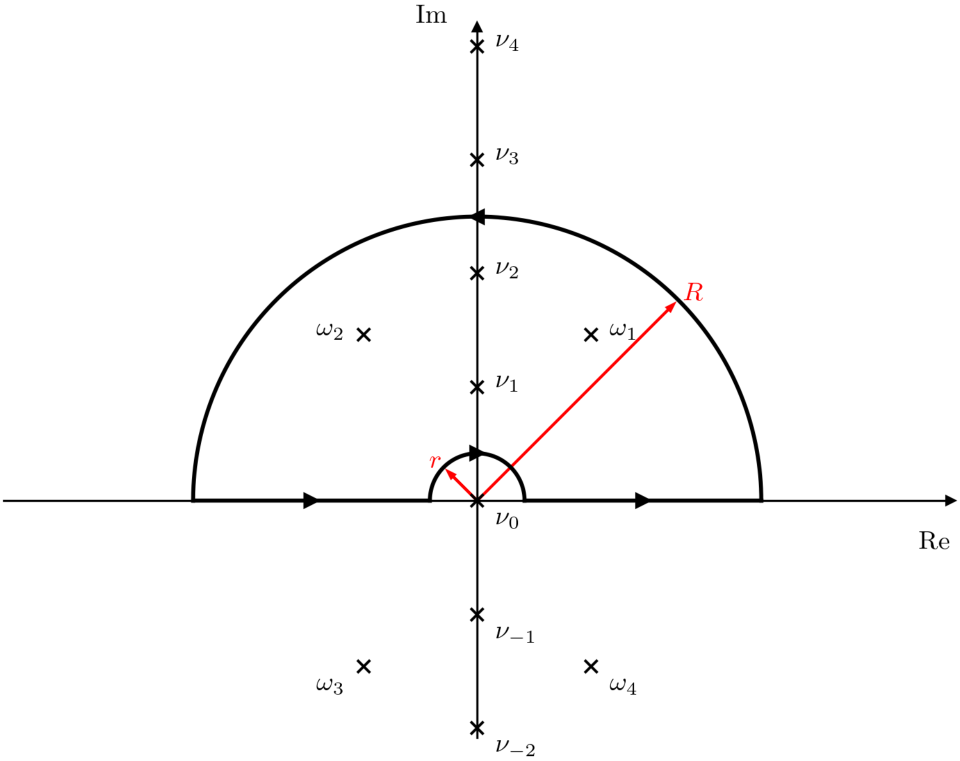
$$\Gamma^{(2)}_{\mu\nu} = \frac{\Delta^2_{\mu\nu}}{4} e^{\bar{Y}+\mathrm{i}\bar{V}} \sum_{m,n=-\infty}^{\infty} \mathrm{i}^m J_m(-\bar{V}+\mathrm{i}\bar{Y}) J_n(\bar{W}+\mathrm{i}\bar{C}) \tag{3.37}$$

$$\int_0^{\infty} \mathrm{d}\tau \Big[1 - \Big(\frac{\bar{A}}{2} + \frac{\bar{V}\Omega}{4}\Big)\tau e^{\mathrm{i}\Omega\tau} - \Big(\frac{\bar{A}}{2} - \frac{\bar{V}\Omega}{4}\Big)\tau e^{-\mathrm{i}\Omega\tau}\Big] e^{\mathrm{i}(m+n)\Omega\tau} + \mathrm{c.c.} \tag{3.38}$$

This expression can be readily integrated to finally give

$$\Gamma^{(2)}_{\mu\nu} = \frac{\Delta^2_{\mu\nu}}{2} \mathrm{Re}\Big\{ e^{\bar{Y}+\mathrm{i}\bar{V}} \sum_{m,n=-\infty}^{\infty} \mathrm{i}^m J_m(-\bar{V}+\mathrm{i}\bar{Y}) J_n(\bar{W}+\mathrm{i}\bar{C}) \times \Big[\frac{1}{\bar{B} - \mathrm{i}(E_{\mu\nu} + \Omega(m+n))} + \tag{3.39}$$

$$+ \frac{\bar{A}/2 + \Omega\bar{V}/4}{(\bar{B} - \mathrm{i}(E_{\mu\nu} + \Omega(m+n+1)))^2} + \frac{\bar{A}/2 + \Omega\bar{V}/4}{(\bar{B} - \mathrm{i}(E_{\mu\nu} + \Omega(m+n-1)))^2}\Big]\Big\}. \tag{3.40}$$



$$
\begin{aligned}
&S(\tau) \\
&= 2\pi\alpha \Bigg[\frac{(\tilde{\Omega}^2+\Gamma^2/4)^2}{2\mathrm{i}\tilde{\Omega}\Gamma(\tilde{\Omega}+\mathrm{i}\Gamma/2)(2\tilde{\Omega}+\mathrm{i}\Gamma)} \coth\left(\frac{\hbar\beta}{2}\left(\tilde{\Omega}+\mathrm{i}\Gamma/2\right)\right)\left(1-e^{\mathrm{i}\tilde{\Omega}\tau}e^{-(\Gamma/2)\tau}\right) \\
&\qquad + \frac{(\tilde{\Omega}^2+\Gamma^2/4)^2}{(-2\mathrm{i}\tilde{\Omega}\Gamma)(-\tilde{\Omega}+\mathrm{i}\Gamma/2)(-2\tilde{\Omega}+\mathrm{i}\Gamma)} \coth\left(\frac{\hbar\beta}{2}\left(-\tilde{\Omega}+\mathrm{i}\Gamma/2\right)\right)\left(1-e^{-\mathrm{i}\tilde{\Omega}\tau}e^{-(\Gamma/2)\tau}\right) \\
&\quad + \frac{2}{\hbar\beta}\sum_{n=1}^{\infty} \frac{(\tilde{\Omega}^2+\Gamma^2/4)^2}{\mathrm{i}\nu_n(\mathrm{i}\nu_n-\tilde{\Omega}-\mathrm{i}\Gamma/2)(\mathrm{i}\nu_n+\tilde{\Omega}-\mathrm{i}\Gamma/2)(\mathrm{i}\nu_n+\tilde{\Omega}+\mathrm{i}\Gamma/2)(\mathrm{i}\nu_n-\tilde{\Omega}+\mathrm{i}\Gamma/2)}(1-e^{-\nu_n\tau}) \Bigg]
\end{aligned}
\tag{3.41}
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4 Chapter 4

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5 Conclusion

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A Appendix

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