Dynamics of the dissipative four-state system

University of Hamburg

Yannic Joshua Banthien

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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 Hamiltonian

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

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

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

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

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

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 $J(\omega) \to 2\alpha\omega$.

3.1 The DW-system in the DVR-basis

Now, we will calculate the form of the single double-well Hamiltonian (3.1) in the DVR-basis. For clarity, we first introduce dimensionless quantities according to

$$\tilde{\mathbf{q}} = \sqrt{\frac{\mathcal{M}\omega_0}{\hbar}}\mathbf{q}, \qquad \tilde{t} = \omega_0 t, \qquad \tilde{T} = \frac{k_B}{\hbar\omega_0}T \tag{3.7}$$

$$\tilde{\Omega} = \frac{\Omega}{\omega_0}, \qquad E_b = \frac{\Delta U}{\hbar\omega_0}, \qquad \tilde{\epsilon} = \sqrt{\frac{1}{\mathcal{M}\hbar\omega_0}}\epsilon. \tag{3.8}$$

The Hamiltonian, in units of $\hbar\omega_0$, now reads

$$\tilde{\mathbf{H}}_{\mathrm{DW}} = \frac{\tilde{\mathbf{p}}^2}{2} + \frac{1}{64E_b}\tilde{\mathbf{q}}^4 - \frac{1}{4}\tilde{\mathbf{q}}^2 - \tilde{\epsilon}\tilde{\mathbf{q}}. \tag{3.9}$$

From now on, we will drop the tildes and only use the rescaled, dimensionless quantities. To obtain the eigenvalues of the position operator and the matrix elements of the double-well Hamiltonian, the procedure described next is peformed. Using the eigenstates $\{|i\rangle\}$ of the simple harmonic oscillator and expressing the position and momentum operators in terms of ladder operators, it is possible to calculate the matrix elements $H^{\mathrm{SHO}}_{\mathrm{DW},mn} = \langle m| \mathbf{H}_{\mathrm{DW}} |n\rangle$, which is in principle an infinite-dimensional square matrix. Since we are mostly interested in the lowest four energy levels, we choose to only keep the $K \times K$ submatrix consisting of the first K rows and column. Naturally, we have to choose K large enough such that the smallest four eigenvalues have converged sufficiently close to their asymptotic value. The resulting $K \times K$ matrix can then be diagonalized using standard analytical or numerical methods, returning K energy eigenvalues $\{\mathcal{E}_1, \mathcal{E}_2, ..., \mathcal{E}_K\}$ and eigenvectors $\{\Psi_1, \Psi_2, ..., \Psi_K\}$. The diagonalized matrix is then obtained as

$$\mathbf{H}^{\mathrm{Eig}}_{\mathrm{DW}} = M_{\mathrm{SHO}\to\mathrm{Eig}}\mathbf{H}^{\mathrm{SHO}}_{\mathrm{DW}} M^{-1}_{\mathrm{SHO}\to\mathrm{Eig}} = \mathrm{diag}(\mathcal{E}_1, \mathcal{E}_2, ..., \mathcal{E}_K), \tag{3.10}$$

with $M_{\mathrm{SHO}\to\mathrm{Eig}}$ being basis transformation matrix whose k-th column is the k-th eigenvector $|\Psi_k\rangle$ in the SHO-basis. Having determined the first K eigenenergies to sufficient precision, we now only keep the four lowest energy eigenstates such that

$$\mathbf{H}^{\mathrm{Eig}}_{\mathrm{DW}} = \mathrm{diag}(\mathcal{E}_1, \mathcal{E}_2, \mathcal{E}_3, \mathcal{E}_4). \tag{3.11}$$

Because we are interested in the evolutions of populations of the left and right side of the wells, we switch to the localized basis defined by

$$|L_1\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle - |\psi_2\rangle\right), \qquad |R_1\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle + |\psi_2\rangle\right), \tag{3.12}$$

$$|L_2\rangle = \frac{1}{\sqrt{2}}\left(|\psi_3\rangle - |\psi_4\rangle\right), \qquad |R_2\rangle = \frac{1}{\sqrt{2}}\left(|\psi_3\rangle + |\psi_4\rangle\right). \tag{3.13}$$

From this definition the basis transformation matrix can be read off to be

$$M_{\mathrm{Eig}\to\mathrm{Loc}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \tag{3.14}$$

and as before, the Hamiltonian in the localized basis is

$$\mathbf{H}^{\mathrm{Loc}}_{\mathrm{DW}} = M_{\mathrm{Eig}\to\mathrm{Loc}}\mathbf{H}^{\mathrm{Eig}}_{\mathrm{DW}} M^{-1}_{\mathrm{Eig}\to\mathrm{Loc}} \tag{3.15}$$

$$= \sum_{i=1,2}\left[\bar{\mathcal{E}}_i(|L_i\rangle\langle L_i| + |R_i\rangle\langle R_i|) - \frac{\Delta_i}{2}(|L_i\rangle\langle R_i| + |R_i\rangle\langle L_i|)\right], \tag{3.16}$$

with $\bar{\mathcal{E}}_1 = (\mathcal{E}_1 + \mathcal{E}_2)/2$, $\bar{\mathcal{E}}_2 = (\mathcal{E}_3 + \mathcal{E}_4)/2$, $\Delta_1 = \mathcal{E}_2 - \mathcal{E}_1$ and $\Delta_2 = \mathcal{E}_4 - \mathcal{E}_3$. One can verify that $\langle\psi_i| \mathbf{q} |\psi_j\rangle = \langle\psi_j| \mathbf{q} |\psi_i\rangle$ and that further $\langle\psi_1| \mathbf{q} |\psi_3\rangle = \langle\psi_2| \mathbf{q} |\psi_4\rangle = 0$, such that one can write the position operator $\mathbf{q}$ in the localized basis as

$$\mathbf{q}^{\mathrm{Loc}} = q_{12}(|R_1\rangle\langle R_1| - |L_1\rangle\langle L_1|) + q_{34}(|R_2\rangle\langle R_2| - |L_2\rangle\langle L_2|) \tag{3.17}$$

$$+ \frac{q_{12} + q_{34}}{2}(|R_1\rangle\langle R_2| + |R_2\rangle\langle R_1| - |L_1\rangle\langle L_2| - |L_2\rangle\langle L_1|) \tag{3.18}$$

$$+ \frac{q_{12} - q_{34}}{2}(|R_2\rangle\langle L_1| + |L_1\rangle\langle R_2| - |L_2\rangle\langle R_1| - |R_1\rangle\langle L_2|) \tag{3.19}$$

Using the representation of the momentum and position operators in terms of the ladder operators of the simple harmonic oscillator,

$$\mathbf{q} = \frac{1}{\sqrt{2}}(\mathbf{a} + \mathbf{a}^\dagger), \qquad \mathbf{p} = \frac{1}{\sqrt{2}\mathrm{i}}(\mathbf{a} - \mathbf{a}^\dagger), \tag{3.20}$$

we can compute the matrix elements of the Hamiltonian in the SHO basis to be

$$\langle m|\mathbf{H}_{\mathrm{DW}}^{\mathrm{SHO}}|n\rangle = \frac{1}{8}\left[(2n+1)\delta_{m,n} - 3\sqrt{n(n-1)}\delta_{m,n-2} - 3\sqrt{(n+1)(n+2)}\delta_{m,n+2}\right] \tag{3.21}$$

$$+ \frac{1}{256E_b}\left[\sqrt{n(n-1)(n-2)(n-3)}\delta_{m,n-4} + 2(2n-1)\sqrt{n(n-1)}\delta_{m,n-2}\right. \tag{3.22}$$

$$+ 3(2n^2+2n+1)\delta_{m,n} + 2(2n+3)\sqrt{(n+1)(n+2)}\delta_{m,n+2} \tag{3.23}$$

$$\left. + \sqrt{(n+1)(n+2)(n+3)(n+4)}\delta_{m,n+4}\right]. \tag{3.24}$$

We then take the submatrix conisting of the first $K \in \mathbb{N}$ rows and columns of $\mathbf{H}_{\mathrm{DW}}^{\mathrm{SHO}}$ and diagonalize it. Since K has to be chosen such that the resulting eigenvalues have converged closely to their actual values and is thus relatively large (e.g. $K = 50$), this has to be done numerically. This yields a set of eigenenergies $\{\mathcal{E}_1, \mathcal{E}_2, ..., \mathcal{E}_K\}$ and corresponding eigenvectors

$$|\psi_i\rangle = \sum_{k=0}^{K-1} c_k^{(i)}\,|k\rangle\,, \tag{3.25}$$

with $|k\rangle$ being the k-th SHO eigenstate and $c_k^{(i)}$ being the entry in the i-th row and k-th column of the basis transformation matrix. Now, we restrict our system to its four lowest energy eigenstates and perform a further basis transformation to the so-called localized basis defined by

$$|L_1\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle - |\psi_2\rangle\right), \qquad |R_1\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle + |\psi_2\rangle\right), \tag{3.26}$$

$$|L_2\rangle = \frac{1}{\sqrt{2}}\left(|\psi_3\rangle - |\psi_4\rangle\right), \qquad |R_2\rangle = \frac{1}{\sqrt{2}}\left(|\psi_3\rangle + |\psi_4\rangle\right). \tag{3.27}$$

The Hamiltonian in the localized basis can be determined by basic matrix algebra, eventually giving

$$\mathbf{H}_{\mathrm{DW}}^{\mathrm{LOC}} = \sum_{i=1,2}\left[\bar{\mathcal{E}}_i(|L_i\rangle\langle L_i| + |R_i\rangle\langle R_i|) - \frac{\Delta_i}{2}(|L_i\rangle\langle R_i| + |R_i\rangle\langle L_i|)\right], \tag{3.28}$$

where $\bar{\mathcal{E}}_1 = (\mathcal{E}_1 + \mathcal{E}_2)/2$, $\bar{\mathcal{E}}_2 = (\mathcal{E}_3 + \mathcal{E}_4)/2$, $\Delta_1 = \mathcal{E}_2 - \mathcal{E}_1$ and $\Delta_2 = \mathcal{E}_4 - \mathcal{E}_3$.

3.2 Calculation of the Rate Matrix Elements

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

$$\Gamma_{\mu\nu}^{(2)} = \frac{\Delta_{\mu\nu}^2}{2}\int_0^\infty \mathrm{d}\tau e^{-(q_\mu - q_\nu)^2 S(\tau)}\cos\left[(E_\mu - E_\nu)\,\tau + (q_\mu - q_\nu)^2\,R\,(\tau)\right], \tag{3.29}$$

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

$$Q\,(\tau) = S\,(\tau) + \mathrm{i}R\,(\tau) = \frac{1}{\pi}\int_0^\infty \mathrm{d}\omega\frac{J\,(\omega)}{\omega^2}\coth\frac{\hbar\omega\beta}{2}\left[(1-\cos\omega\tau) + \mathrm{i}\sin\omega\tau\right]. \tag{3.30}$$

Again, as in the section before, we use dimensionless quantities as defined previously, in addition of $\tilde{\Gamma} = \Gamma/\omega_0$. 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

$$S\,(\tau) + \mathrm{i}R\,(\tau) = \frac{2\alpha}{\pi}\int_0^\infty \mathrm{d}\omega\frac{1}{\omega}\frac{\Omega^4}{(\Omega^2-\omega^2)^2 + (\Gamma\omega)^2}\coth\frac{\hbar\omega\beta}{2}\left[(1-\cos\omega\tau) + \mathrm{i}\sin\omega\tau\right]. \tag{3.31}$$

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

$$S(\tau) = \frac{2\alpha}{\pi}\int_0^\infty \mathrm{d}\omega \frac{1}{\omega}\frac{\Omega^4}{\left(\Omega^2-\omega^2\right)^2+(\Gamma\omega)^2}\coth\frac{\hbar\omega\beta}{2}\left(1-\cos\omega\tau\right). \tag{3.32}$$

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

$$S(\tau) = \frac{\alpha}{\pi}\int_{-\infty}^\infty \mathrm{d}\omega \frac{1}{\omega}\frac{\Omega^4}{\left(\Omega^2-\omega^2\right)^2+(\Gamma\omega)^2}\coth\frac{\hbar\omega\beta}{2}\left(1-e^{\mathrm{i}\omega\tau}\right). \tag{3.33}$$

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

$$\left(\Omega^2-\omega^2\right)^2+(\Gamma\omega)^2 = 0. \tag{3.34}$$

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

$$\omega_{1,2,3,4} = \pm\frac{\mathrm{i}\Gamma}{2} \pm \sqrt{\frac{\Gamma^2}{4}+\Omega^2} = \pm\bar{\Omega} \pm \frac{\mathrm{i}\Gamma}{2}, \tag{3.35}$$

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

$$\omega = \mathrm{i}\frac{2\pi k}{\hbar\beta} = \mathrm{i}\nu_k,\ \ k \in \mathbb{Z}, \tag{3.36}$$

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

$$\int_{-\infty}^\infty \mathrm{d}\omega F(\omega) = 2\pi\mathrm{i}\sum_k \mathrm{Res}(F,\omega_k) - \lim_{R\to\infty}\int_{\mathcal{C}_1}\mathrm{d}\omega F(\omega) - \lim_{r\to 0}\int_{\mathcal{C}_2}\mathrm{d}\omega F(\omega), \tag{3.37}$$

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

$$S(\tau) = X\tau + L\left(e^{-(\Gamma/2)\tau}\cos\bar{\Omega}\tau - 1\right) + Ze^{-(\Gamma/2)\tau}\sin\bar{\Omega}\tau + S_{\mathrm{Mats}}(\tau), \tag{3.38}$$

with the prefactors being

$$L = \frac{\alpha}{\Gamma\bar{\Omega}}\frac{1}{\cosh(\hbar\beta\bar{\Omega})-\cos(\hbar\beta\Gamma/2)}\left[\left(\frac{\Gamma^2}{4}-\bar{\Omega}^2\right)\sinh(\hbar\beta\bar{\Omega}) + \Gamma\bar{\Omega}\sin(\hbar\beta\Gamma/2)\right], \tag{3.39}$$

$$Z = \frac{\alpha}{\Gamma\bar{\Omega}}\frac{1}{\cosh(\hbar\beta\bar{\Omega})-\cos(\hbar\beta\Gamma/2)}\left[-\Gamma\bar{\Omega}\sinh(\hbar\beta\bar{\Omega}) + \left(\frac{\Gamma^2}{4}-\bar{\Omega}^2\right)\sin(\hbar\beta\Gamma/2)\right], \tag{3.40}$$

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

$$S_{\mathrm{Mats}}(\tau) = -\frac{4\alpha\Omega^4}{\hbar\beta}\sum_{n=1}^\infty \frac{1}{(\Omega^2+\nu_n^2)^2-\Gamma^2\nu_n^2}\left[\frac{e^{-\nu_n\tau}-1}{\nu_n}\right]. \tag{3.41}$$

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

$$R(\tau) = \frac{2\alpha}{\pi}\int_0^\infty \mathrm{d}\omega \frac{1}{\omega}\frac{\Omega^4}{\left(\Omega^2-\omega^2\right)^2+(\Gamma\omega)^2}\sin\omega\tau \tag{3.42}$$

$$= \frac{\alpha}{\pi}\int_{-\infty}^\infty \mathrm{d}\omega \frac{1}{\omega}\frac{\Omega^4}{\left(\Omega^2-\omega^2\right)^2+(\Gamma\omega)^2}e^{\mathrm{i}\omega\tau}, \tag{3.43}$$

the imaginary part can be analogously computed to be

$$R(\tau) = \alpha - \alpha e^{-(\Gamma/2)\tau}\left(N\sin\bar{\Omega}\tau + \cos\bar{\Omega}\tau\right), \tag{3.44}$$

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

$$S(\tau) = Y(\cos\Omega\tau - 1) + A\tau\cos\Omega\tau + B\tau\sin\Omega\tau + \mathcal{O}\left[\kappa^2\right], \tag{3.45}$$

$$R(\tau) = W\sin\Omega\tau + V(1-\cos\Omega\tau - \frac{\Omega}{2}\tau\sin\Omega\tau) + \mathcal{O}\left[\kappa^2\right], \tag{3.46}$$

with the temperature dependent coefficients

$$Y = -\frac{4g^2}{\Omega^2}\coth\frac{\hbar\beta\Omega}{2}, \quad W = \frac{4g^2}{\Omega^2} \tag{3.47}$$

$$A = \frac{4\Gamma g^2}{2\Omega^2}\coth\frac{\hbar\beta\Omega}{2}, \quad B = \frac{8\Gamma g^2}{\Omega^2\hbar\beta} \tag{3.48}$$

$$C = -\frac{2\Gamma g^2}{\Omega^3}\frac{\hbar\beta\Omega + 2\sinh\hbar\beta\Omega}{\cosh\hbar\beta\Omega - 1}, \quad V = \frac{4\Gamma g^2}{\Omega^3}. \tag{3.49}$$

We now turn to the computation of the rate matrix elements. Inserting the real and imaginary parts of the bath correlation function into (3.29), we obtain

$$\begin{aligned}\Gamma^{(2)}_{\mu\nu} = \frac{\Delta^2_{\mu\nu}}{2}\int_0^\infty &\mathrm{d}\tau \exp\Big\{-q^2_{\mu\nu}Y(\cos\Omega\tau - 1) - q^2_{\mu\nu}A\tau\cos\Omega\tau - q^2_{\mu\nu}B\tau\cos\Omega\tau\Big\} \\ &\times\cos\Big\{E_{\mu\nu}\tau + q^2_{\mu\nu}W\sin\Omega\tau + V\Big(1-\cos\Omega\tau - \frac{\Omega}{2}\tau\sin\Omega\tau\Big)\Big\},\end{aligned} \tag{3.50}$$

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

$$\Gamma^{(2)}_{\mu\nu} = \frac{\Delta^2_{\mu\nu}}{4}e^{\bar{Y}+\mathrm{i}\bar{V}}\int_0^\infty \mathrm{d}\tau e^{-\bar{B}\tau - \bar{A}\tau\cos\omega\tau}e^{\mathrm{i}E_{\mu\nu}\tau - \mathrm{i}\bar{V}\frac{\Omega}{2}\tau\sin\omega\tau}e^{(-\bar{Y}-\mathrm{i}\bar{V})\cos\omega\tau}e^{(-\bar{C}+\mathrm{i}\bar{W})\sin\omega\tau} + \mathrm{c.c} \tag{3.51}$$

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

$$\frac{4}{\hbar\beta\Omega} > \coth\frac{\hbar\beta\Omega}{2}. \tag{3.52}$$

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

$$e^{-\bar{A}\tau\cos\omega\tau} \approx 1 - \bar{A}\tau\cos\omega\tau \tag{3.53}$$

$$e^{-\mathrm{i}\bar{V}\frac{\Omega}{2}\tau\sin\omega\tau} \approx 1 - \mathrm{i}\bar{V}\frac{\Omega}{2}\tau\sin\omega\tau. \tag{3.54}$$

Further, we estimate the product of these linearized terms as

$$\Big(1-\bar{A}\tau\cos\omega\tau\Big)\Big(1-\mathrm{i}\bar{V}\frac{\Omega}{2}\tau\sin\omega\tau\Big) \approx 1 - \Big(\frac{\bar{A}}{2}+\frac{\bar{V}\Omega}{4}\Big)\tau e^{\mathrm{i}\Omega\tau} - \Big(\frac{\bar{A}}{2}-\frac{\bar{V}\Omega}{4}\Big)\tau e^{-\mathrm{i}\Omega\tau}. \tag{3.55}$$

Employing the Jacobi-Anger expansions

$$e^{\mathrm{i}z\cos\theta} = \sum_{n=-\infty}^{\infty} \mathrm{i}^n J_n(z) e^{\mathrm{i}n\theta} \tag{3.56}$$

and respectively

$$e^{\mathrm{i}z\sin\theta} = \sum_{n=-\infty}^{\infty} J_n(z) e^{\mathrm{i}n\theta}, \tag{3.57}$$

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

$$e^{(-\bar{Y}-\mathrm{i}\bar{V})\cos\omega\tau} e^{(-\bar{C}+\mathrm{i}\bar{W})\sin\omega\tau} = \sum_{m,n=-\infty}^{\infty} \mathrm{i}^m J_m(-\bar{V}+\mathrm{i}\bar{Y}) J_n(\bar{W}+\mathrm{i}\bar{C}) e^{\mathrm{i}(m+n)\Omega\tau}. \tag{3.58}$$

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

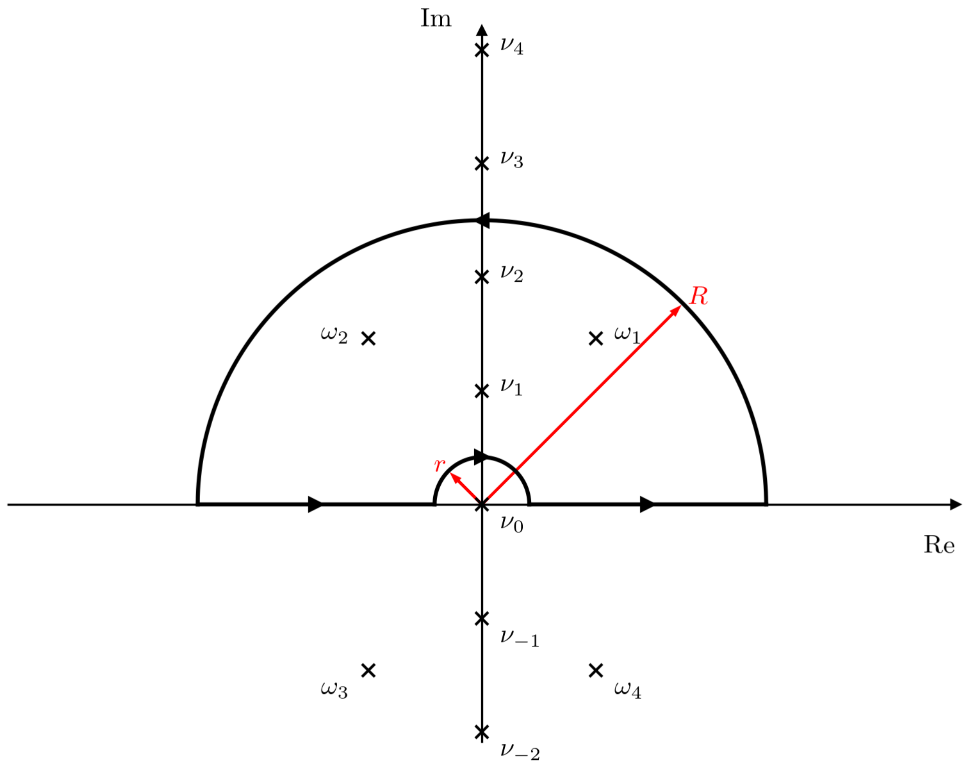
$$\Gamma^{(2)}_{\mu\nu} = \frac{\Delta^2_{\mu\nu}}{4} e^{\bar{Y}+\mathrm{i}\bar{V}} \sum_{m,n=-\infty}^{\infty} \mathrm{i}^m J_m(-\bar{V}+\mathrm{i}\bar{Y}) J_n(\bar{W}+\mathrm{i}\bar{C}) \tag{3.59}$$

$$\int_0^\infty \mathrm{d}\tau \Big[1 - \Big(\frac{\bar{A}}{2} + \frac{\bar{V}\Omega}{4}\Big)\tau e^{\mathrm{i}\Omega\tau} - \Big(\frac{\bar{A}}{2} - \frac{\bar{V}\Omega}{4}\Big)\tau e^{-\mathrm{i}\Omega\tau}\Big] e^{\mathrm{i}(m+n)\Omega\tau} + \text{c.c.} \tag{3.60}$$

This expression can be readily integrated to finally give

$$\Gamma^{(2)}_{\mu\nu} = \frac{\Delta^2_{\mu\nu}}{2} \mathrm{Re}\Big\{ e^{\bar{Y}+\mathrm{i}\bar{V}} \sum_{m,n=-\infty}^{\infty} \mathrm{i}^m J_m(-\bar{V}+\mathrm{i}\bar{Y}) J_n(\bar{W}+\mathrm{i}\bar{C}) \times \Big[\frac{1}{\bar{B}-\mathrm{i}(E_{\mu\nu}+\Omega(m+n))} + \tag{3.61}$$

$$+ \frac{\bar{A}/2+\Omega\bar{V}/4}{(\bar{B}-\mathrm{i}(E_{\mu\nu}+\Omega(m+n+1)))^2} + \frac{\bar{A}/2+\Omega\bar{V}/4}{(\bar{B}-\mathrm{i}(E_{\mu\nu}+\Omega(m+n-1)))^2}\Big]\Big\}. \tag{3.62}$$



$$
\begin{aligned}
&S(\tau) \\
&= 2\pi\alpha \left[\frac{(\tilde{\Omega}^2 + \Gamma^2/4)^2}{2\mathrm{i}\tilde{\Omega}\Gamma(\tilde{\Omega} + \mathrm{i}\Gamma/2)(2\tilde{\Omega} + \mathrm{i}\Gamma)} \coth\left(\frac{\hbar\beta}{2}\left(\tilde{\Omega} + \mathrm{i}\Gamma/2\right)\right)\left(1 - e^{\mathrm{i}\tilde{\Omega}\tau} e^{-(\Gamma/2)\tau}\right) \right. \\
&\qquad\qquad + \frac{(\tilde{\Omega}^2 + \Gamma^2/4)^2}{(-2\mathrm{i}\tilde{\Omega}\Gamma)(-\tilde{\Omega} + \mathrm{i}\Gamma/2)(-2\tilde{\Omega} + \mathrm{i}\Gamma)} \coth\left(\frac{\hbar\beta}{2}\left(-\tilde{\Omega} + \mathrm{i}\Gamma/2\right)\right)\left(1 - e^{-\mathrm{i}\tilde{\Omega}\tau} e^{-(\Gamma/2)\tau}\right) \\
&\quad \left. + \frac{2}{\hbar\beta} \sum_{n=1}^{\infty} \frac{(\tilde{\Omega}^2 + \Gamma^2/4)^2}{\mathrm{i}\nu_n(\mathrm{i}\nu_n - \tilde{\Omega} - \mathrm{i}\Gamma/2)(\mathrm{i}\nu_n + \tilde{\Omega} - \mathrm{i}\Gamma/2)(\mathrm{i}\nu_n + \tilde{\Omega} + \mathrm{i}\Gamma/2)(\mathrm{i}\nu_n - \tilde{\Omega} + \mathrm{i}\Gamma/2)} (1 - e^{-\nu_n\tau}) \right]
\end{aligned} \tag{3.63}
$$

4 Chapter 4

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5 Conclusion

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A Appendix

We want to evaluate the integral

$$
\begin{aligned}
Q(\tau) &= \frac{1}{\pi}\int_0^\infty \mathrm{d}\omega \frac{J(\omega)}{\omega^2}\coth\frac{\hbar\omega\beta}{2}\Big[(1-\cos\omega\tau)+\mathrm{i}\sin\omega\tau\Big] \\
&= \frac{\alpha}{\pi}\int_{-\infty}^\infty \mathrm{d}\omega \frac{1}{\omega}\frac{\Omega^4}{\left(\Omega^2-\omega^2\right)^2+(\Gamma\omega)^2}\coth\frac{\hbar\omega\beta}{2}\Big[(1-\cos\omega\tau)+\mathrm{i}\sin\omega\tau\Big] \\
&= \frac{\alpha}{\pi}\int_{-\infty}^\infty \mathrm{d}\omega \frac{1}{\omega}\frac{\Omega^4}{\left(\Omega^2-\omega^2\right)^2+(\Gamma\omega)^2}\coth\frac{\hbar\omega\beta}{2}\Big[\left(1-e^{\mathrm{i}\omega\tau}\right)+\mathrm{i}e^{\mathrm{i}\omega\tau}\Big].
\end{aligned}
\tag{A.1}
$$

via the use of the residue theorem. To this end, we continue the integrand analytically and examine it for poles. For clarity, we will consider the real part and the imaginary part seperately. The real part of (A.1) reads

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

The first factor has poles at the solutions of

$$
\left(\Omega^2-\omega^2\right)^2+(\Gamma\omega)^2 = 0. \tag{A.3}
$$

Solving this equation is done by simple algebra, revealing four simple poles at

$$
\omega = \pm\frac{\mathrm{i}\Gamma}{2}\pm\sqrt{\frac{\Gamma^2}{4}+\Omega^2} = \pm\bar{\Omega}\pm\frac{\mathrm{i}\Gamma}{2}. \tag{A.4}
$$

The second factor does not possess any poles, since

$$
\lim_{z\to 0}\frac{1-e^{\mathrm{i}z\tau}}{z} = -\mathrm{i}\tau. \tag{A.5}
$$

The third factor has simple poles at the zeroes of the complex sine function, which are at $z = \mathrm{i}k\pi$ for $k\in\mathbb{Z}$. The poles are therefore at

$$
\frac{\hbar\omega\beta}{2} = \mathrm{i}k\pi \Leftrightarrow \omega = \mathrm{i}\frac{2\pi k}{\hbar\beta}, \tag{A.6}
$$

which are the bosonic Matsubara frequencies. Having identified all poles, we now have to choose a suitable integration contour. In this case, we will choose the half-annulus lying in the upper complex half-plane with inner radius r and outer radius R traversed in the mathematically positive sense. In the limit $R\to\infty$ and $r\to 0$, this contour encircles the two poles of the first factor that lie in the upper half-plane as well as all the poles of the hyperbolic cotangent for which $k>0$. With this contour, our integral takes the form

$$
\int_{-\infty}^\infty \mathrm{d}\omega F(\omega) = 2\pi\mathrm{i}\sum_k \mathrm{Res}(F,\omega_k) - \lim_{r\to 0}\int_{\mathcal{C}_2}\mathrm{d}\omega F(\omega), \tag{A.7}
$$

where $\mathcal{C}_2$ denotes the inner half-circle and $\{\omega_k\}_{k\in I}$ is the set of all encircled poles. First, we will compute the terms coming from the integration over the inner half-circle:

$$\begin{aligned}\lim_{r\to 0}\int_{\mathcal{C}_2} \mathrm{d}\omega F(\omega) &= \frac{\mathrm{i}\alpha}{\pi}\int_{\pi}^{0}\mathrm{d}\phi \lim_{r\to 0}\frac{\Omega^4}{(\Omega^2 - r^2 e^{i2\phi})^2 + (\Gamma r e^{i\phi})^2}\left(1 - e^{\mathrm{i}re^{i\phi}\tau}\right)\coth\frac{\hbar r e^{i\phi}\beta}{2} \\ &= -\frac{\mathrm{i}\alpha}{\pi}\frac{2\mathrm{i}\tau}{\hbar\beta}\int_{\pi}^{0}\mathrm{d}\phi \\ &= -\frac{2\alpha}{\hbar\beta}\tau.\end{aligned} \tag{A.8}$$

The residue at the simple pole ω_k is calculated through the formula

$$\mathrm{Res}(F,\omega_k) = \lim_{\omega\to\omega_k}(\omega - \omega_k)F(\omega). \tag{A.9}$$

At the pole $\omega = \bar{\Omega} + \mathrm{i}\Gamma/2$, this amount to

$$\mathrm{Res}(F,\bar{\Omega} + \mathrm{i}\Gamma/2) = -\frac{\mathrm{i}\alpha}{\pi}\left[\frac{\bar{\Omega}^2 - \Gamma^2/4}{4\bar{\Omega}\Gamma} - \frac{\mathrm{i}}{4}\right]\frac{\sinh\hbar\beta\bar{\Omega} - \mathrm{i}\sin\hbar\beta\Gamma/2}{\cosh\hbar\beta\bar{\Omega} - \cos\hbar\beta\Gamma/2}(1 - e^{\mathrm{i}\bar{\Omega}\tau}e^{-\Gamma/2\tau}) \tag{A.10}$$

and conversely for $\omega = -\bar{\Omega} + \mathrm{i}\Gamma/2$

$$\mathrm{Res}(F,-\bar{\Omega} + \mathrm{i}\Gamma/2) = -\frac{\mathrm{i}\alpha}{\pi}\left[\frac{\bar{\Omega}^2 - \Gamma^2/4}{4\bar{\Omega}\Gamma} + \frac{\mathrm{i}}{4}\right]\frac{\sinh\hbar\beta\bar{\Omega} + \mathrm{i}\sin\hbar\beta\Gamma/2}{\cosh\hbar\beta\bar{\Omega} - \cos\hbar\beta\Gamma/2}(1 - e^{-\mathrm{i}\bar{\Omega}\tau}e^{-\Gamma/2\tau}). \tag{A.11}$$