Cavity Polaritronics

Yannic Joshua Banthien[1]

[1] *Universität Hamburg*

(November 14, 2024)

These notes serve to document the developements of the masters thesis of Yannic Joshua Banthien written in 2024 and 2025.

I. INTRODUCTION

We want to consider the dynamics of N identical doublet-doublet systems, each coupled to a single cavity mode, which in turn is coupled to a bath of harmonic oscillators. For this model, the full Hamiltonian is given by

$$\mathbf{H} = \sum_{j=1}^{N} \mathbf{H}_{\mathrm{DW,j}} + \mathbf{H}_{\mathrm{C,int}} + \mathbf{H}_{\mathrm{B,int}}, \tag{1}$$

where

$$\mathbf{H}_{\mathrm{DW,j}} = \frac{\mathbf{p}_j^2}{2\mathcal{M}} + \frac{\mathcal{M}^2\omega_0^4}{64\Delta U}\mathbf{q}_j^4 - \frac{\mathcal{M}\omega_0^2}{4}\mathbf{q}_j^2 - \mathbf{q}_j\varepsilon, \tag{2}$$

with

$$\mathbf{H}_{\mathrm{C,int}} = \frac{\mathbf{p}_y^2}{2M} + \frac{1}{2}M\Omega^2\mathbf{y}^2 + \sum_{j=1}^{N} gM\Omega^2\mathbf{y}\mathbf{q}_j, \tag{3}$$

and

$$\mathbf{H}_{\mathrm{B,int}} = \sum_{\alpha}\left[\frac{\mathbf{p}_\alpha^2}{2m_\alpha} + \frac{1}{2}m_\alpha\omega_\alpha^2\left\{\mathbf{x}_\alpha + \frac{c_\alpha}{m_\alpha\omega_\alpha^2}\mathbf{y}\right\}^2\right]. \tag{4}$$

Here, $\mathbf{y}$ denotes the coordinate of the cavity mode and the $\mathbf{x}_\alpha$ are the coordinates of the bath oscillators.

II. THE DOUBLET-DOUBLET SYSTEM

We first turn to the single, bare double-well system governed by the Hamiltonian

$$\mathbf{H}_{\mathrm{DW}} = \frac{\mathbf{p}^2}{2\mathcal{M}} + \frac{\mathcal{M}^2\omega_0^4}{64\Delta U}\mathbf{q}^4 - \frac{\mathcal{M}\omega_0^2}{4}\mathbf{q}^2 - \mathbf{q}\varepsilon, \tag{5}$$

where ΔU is the barrier height and ε is the bias of the double-well. Further, we will introduce dimensionless quantities via

$$\begin{aligned} \tilde{t} = \omega_0 t, \qquad \tilde{\mathbf{q}} = \sqrt{\mathcal{M}\omega_0/\hbar}\,\mathbf{q}, \quad \tilde{\mathbf{p}} = \sqrt{1/\mathcal{M}\hbar\omega_0}\,\mathbf{p}, \\ E_{\mathrm{B}} = \Delta U/\omega_0,\ \tilde{\varepsilon} = \sqrt{1/\mathcal{M}\hbar\omega_0^3}\,\varepsilon,\ \tilde{\mathbf{H}}_{\mathrm{DW}} = 1/\hbar\omega_0 \mathbf{H}_{\mathrm{DW}}. \end{aligned} \tag{6}$$

The dimensionless Hamiltonian in units of $\hbar\omega_0$, omitting the tildes, now reads

$$\mathbf{H}_{\mathrm{DW}} = \frac{1}{2}\mathbf{p}^2 + \frac{1}{64E_{\mathrm{B}}}\mathbf{q}^4 - \frac{1}{4}\mathbf{q}^2 - \mathbf{q}\varepsilon. \tag{7}$$

For the sake of brevity, we set $\varepsilon = 0$ in the following discussion. Diagonalization of $\mathbf{H}_{\mathrm{DW}}$ results in a set of energy eigenvalues and eigenstates

$$\{\mathcal{E}_j, |j\rangle\}_{j\in J}\,, \tag{8}$$

with $J = \{1, 2, 3, ...\}$. As we are interested in the dynamics of the lowest doublet-doublet pair, we pick our basis to be the states $\{|1\rangle\,, |2\rangle\,, |3\rangle\,, |4\rangle\}$. From this, we build the so-called localized basis defined as

$$\begin{aligned} |L_1\rangle = 1/\sqrt{2}\left(|1\rangle - |2\rangle\right), \quad |L_2\rangle = 1/\sqrt{2}\left(|1\rangle + |2\rangle\right) \\ |R_1\rangle = 1/\sqrt{2}\left(|3\rangle - |4\rangle\right), \ |R_2\rangle = 1/\sqrt{2}\left(|3\rangle + |4\rangle\right). \end{aligned} \tag{9}$$

Using these relations, it is easy to calculate the Hamiltonian of the isolated doublet-doublet system in the localized basis,

$$\mathbf{H}_{\mathrm{DDS}}^{\mathrm{loc}} = \sum_{i=1,2} \left[\bar{\mathcal{E}}_i \left(|L_i\rangle \langle L_i| + |R_i\rangle \langle R_i| \right) - \frac{\Delta_i}{2} \left(|L_i\rangle \langle R_i| + |R_i\rangle \langle L_i| \right) \right], \tag{10}$$

with the mean intra-doublet energies $\bar{\mathcal{E}}_1 = (\mathcal{E}_1 + \mathcal{E}_2)/2$, $\bar{\mathcal{E}}_2 = (\mathcal{E}_3 + \mathcal{E}_4)/2$ and intra-doublet energy gaps $\Delta_1 = \mathcal{E}_2 - \mathcal{E}_1$, $\Delta_1 = \mathcal{E}_4 - \mathcal{E}_3$. Similary, the position operator in the localized can be calculated to be

$$\begin{aligned} \mathbf{q}^{\mathrm{loc}} = &\sum_{i=1,2} q_i \left(|R_i\rangle \langle R_i| - |L_i\rangle \langle L_i| \right) \\ &+ \bar{q} \left(|L_1\rangle \langle L_2| + |L_2\rangle \langle L_1| + |R_1\rangle \langle R_2| + |R_2\rangle \langle R_1| \right) \\ &+ \frac{\Delta q}{2} \left(|L_1\rangle \langle R_2| + |R_2\rangle \langle L_1| - |R_1\rangle \langle L_2| - |L_2\rangle \langle R_1| \right), \end{aligned} \tag{11}$$

where $q_1 = \langle 1| \mathbf{q} |2\rangle$, $q_2 = \langle 3| \mathbf{q} |4\rangle$, $\bar{q} = (\langle 1| \mathbf{q} |4\rangle + \langle 2| \mathbf{q} |3\rangle)/2$ and $\Delta q = \langle 1| \mathbf{q} |4\rangle - \langle 2| \mathbf{q} |3\rangle$.

Since we are after the position eigenvalues, we next diagonalize the matrix (11). Analytically, this is not possible for the full expression. But, using $\Delta q/2 \ll q_i, \bar{q}$ and noticing that (11) is symmetric, we can make the approximation that $\Delta q/2 = 0$, which allow us to continue the analytical calculation. Carrying out the usual diagonalization process, the eigenstates

$$\begin{aligned} |\alpha_1\rangle &= v \left(|L_1\rangle - u \, |L_2\rangle \right), \;\; |\beta_1\rangle = v \left(|R_1\rangle + u \, |R_2\rangle \right) \\ |\alpha_2\rangle &= v \left(u \, |L_1\rangle + |L_2\rangle \right), \;\; |\beta_2\rangle = v \left(u \, |R_1\rangle + |R_2\rangle \right) \end{aligned} \tag{12}$$

are calculated, with $v = 1/\sqrt{1+u^2}$, $u = (q_1 + q_{\alpha_1})/\bar{q} = -(q_2 + q_{\alpha_2})/\bar{q}$ and $q_{\alpha_i} = -q_{\beta_i}$. The q_{α_i} and q_{β_i} are the position eigenvalues of the position eigenstates localized in the left and respectively right hand side of the double-well, given by

$$q_{\alpha_{1,2}} = \left[(q_1 + q_2) \mp \sqrt{(q_1 - q_2)^2 + 4\bar{q}^2} \right] /2. \tag{13}$$

Transforming to the DVR-basis defined by (12) then finally yields the Hamiltonian in the DVR-basis,

$$\begin{aligned} \mathbf{H}_{\mathrm{DDS}}^{\mathrm{DVR}} = &- \sum_{i,j=1,2} \frac{\Delta_{\alpha_i\beta_j}}{2} (|\alpha_i\rangle \langle\beta_j| + |\beta_j\rangle \langle\alpha_i|) \\ &+ \sum_{i=1,2} (E_{\alpha_i} |\alpha_i\rangle \langle\alpha_i| + E_{\beta_i} |\beta_i\rangle \langle\beta_i|) \\ &- \frac{\Delta_R}{2} (|\alpha_1\rangle \langle\alpha_2| + |\alpha_2\rangle \langle\alpha_1| + |\beta_1\rangle \langle\beta_2| + |\beta_2\rangle \langle\beta_1|). \end{aligned} \tag{14}$$

The off-diagonal matrix elements are then

$$\begin{aligned} \Delta_{\alpha_1\beta_1} &= v^2(\Delta_1 + u^2\Delta_2) \\ \Delta_{\alpha_2\beta_2} &= v^2(u^2\Delta_1 + \Delta_2) \\ \Delta_{\alpha_1\beta_2} &= \Delta_{\alpha_2\beta_1} = uv^2(\Delta_1 - \Delta_2) \\ \Delta_R &= uv^2\bar{\omega}_0, \end{aligned} \tag{15}$$

where $\bar{\omega}_0 = \bar{\mathcal{E}}_2 - \bar{\mathcal{E}}_1$. The matrix elements of the Hamiltonian in the DVR-representation given by (14) together with the position eigenvalues as in (13) are the data needed to continue our analysis. In Fig.1, the wavefunctions of the four states is depicted in different representations.

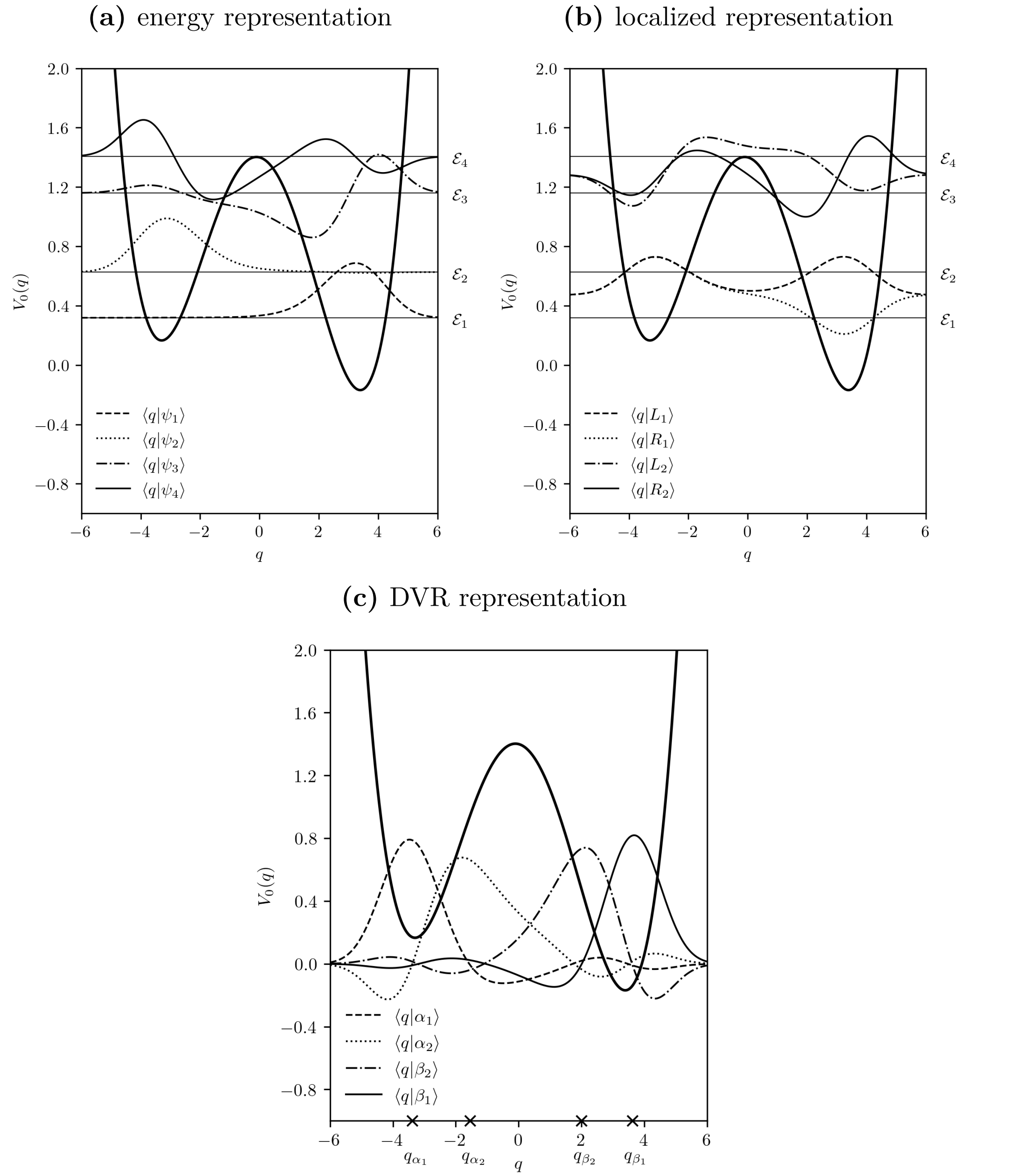

FIG. 1: The first four states in the (a) energy basis, (b) localized basis and (c) DVR basis. Here, a barrier height of $E_b = 1.4$ and a bias of $\varepsilon = 0.05$ are chosen.

III. THE BATH CORRELATION FUNCTION

Next, we calculate the bath correlation function, defined by

$$Q(t) = S(t) + \mathrm{i}R(t) = \frac{1}{\pi}\int_0^\infty \mathrm{d}\omega \frac{J(\omega)}{\omega^2}\left\{\coth\frac{\omega}{2T}(1-\cos\omega t) + \mathrm{i}\sin\omega t\right\}. \tag{16}$$

The effective bath spectral density considered for our purposes will be given by

$$J_{\mathrm{eff}}(\omega) = \frac{2\alpha\Omega^4\omega}{(\Omega^2-\omega^2)^2+(\Gamma\omega)^2}, \tag{17}$$

a Lorentzian spectral density peaked at Ω and width Γ. For clarity, we start with evaluating the real part of (16) and rewrite

$$\begin{aligned} S(t) &= \frac{2\alpha\Omega^4}{\pi}\int_0^\infty \mathrm{d}\omega\frac{1}{\omega}\frac{1}{(\Omega^2-\omega^2)^2+(\Gamma\omega)^2}\coth\frac{\omega}{2T}(1-\cos\omega t) \\ &= \frac{\alpha\Omega^4}{\pi}\int_{-\infty}^{+\infty} \mathrm{d}\omega\frac{1}{\omega}\frac{1}{(\Omega^2-\omega^2)^2+(\Gamma\omega)^2}\coth\frac{\omega}{2T}(1-\exp\mathrm{i}\omega t). \end{aligned} \tag{18}$$

We can evaluate this integral using the residue theorem. To this end, we identify the poles of the first two factors to be $\omega = 0$ and $\omega = \omega_i$, $i = 1,2,3,4$, where

$$\begin{aligned} \omega_1 = \bar{\Omega} + \mathrm{i}\Gamma/2, \quad \omega_2 = -\bar{\Omega} + \mathrm{i}\Gamma/2 \\ \omega_3 = -\bar{\Omega} - \mathrm{i}\Gamma/2, \quad \omega_4 = \bar{\Omega} - \mathrm{i}\Gamma/2 \end{aligned} \tag{19}$$

and $\bar{\Omega} = \sqrt{\Omega^2 - \Gamma^2/4}$. Further, the poles of the cotangent hyperbolicus are

$$\frac{\omega}{2T} \Leftrightarrow \omega = \mathrm{i}2\pi T n = \mathrm{i}\nu_n,\ n \in \mathbb{Z}, \tag{20}$$

with the ν_n being the familiar Matsubara frequencies. The integration contour of choice will be a half annulus bounded by circles of radius r and R, centered at the origin. Then, the limits $r \to 0$ and $R \to \infty$ are taken, returning the sought for integral.

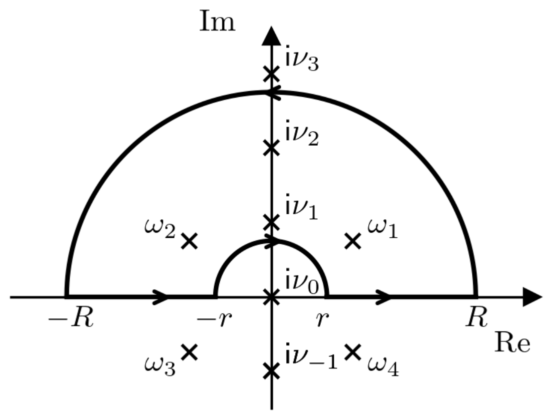

FIG. 2: Integration contour used to evaluate the integral (18).

Carrying out the calculation then finally gives

$$S(t) = Xt + L(e^{-(\Gamma/2)t}\cos\bar{\Omega}t - 1) + Ze^{-(\Gamma/2)t}\sin\bar{\Omega}t + S_{\mathrm{Mats}}(t), \tag{21}$$

where

$$X = 2\alpha T \tag{22}$$

$$L = \frac{\alpha}{\Gamma\bar{\Omega}}\frac{(\Gamma^2/4 - \bar{\Omega}^2)\sinh\bar{\Omega}/T + \Gamma\bar{\Omega}\sin\Gamma/(2T)}{\cosh\bar{\Omega}/T - \cos\Gamma/(2T)} \tag{23}$$

$$Z = \frac{\alpha}{\Gamma\bar{\Omega}}\frac{-\Gamma\bar{\Omega}\sinh\bar{\Omega}/T + (\Gamma^2/4 - \bar{\Omega}^2)\sin\Gamma/(2T)}{\cosh\bar{\Omega}/T - \cos\Gamma/(2T)}. \tag{24}$$

The last term $S_{\mathrm{Mats}}(t)$ is a function of the Matsubara frequencies,

$$S_{\mathrm{Mats}}(t) = -4\alpha\Omega^4 T \sum_{n=1}^{\infty} \frac{1}{(\Omega^2+\nu_n^2)^2 - \Gamma^2\nu_n^2} \Big(\frac{\exp(-\nu_n t) - 1}{\nu_n} \Big). \tag{25}$$

In the regime of $T > \Gamma/(2\pi)$, this term can be neglected, as we will. An analogous calculation for the imaginary part of (16) yields

$$R(t) = \alpha - \alpha e^{-(\Gamma/2)t}(N \sin\bar{\Omega}t + \cos\bar{\Omega}t), \tag{26}$$

where $N = (\Gamma^2/4 - \bar{\Omega}^2)/(\Gamma\bar{\Omega})$. In order to derive an analytical expression for the rate matrix elements, we will employ the so-called weak-damping approximation (WDA). Since we are interested in the case of a sharpely peaked bath spectral density, meaning that $\kappa = \Gamma/(2\pi\Omega) \ll 1$, we may expand the bath correlation function to first order in κ. This procedure gives the result

$$S(\tau) = Y(\cos\Omega\tau - 1) + A\tau\cos\Omega\tau + B\tau + C\sin\Omega\tau + \mathcal{O}(\kappa^2) \tag{27}$$

$$R(\tau) = W\sin\Omega\tau + V\left(1 - \cos\Omega\tau - \frac{\Omega}{2}\tau\sin\Omega\tau\right) + \mathcal{O}(\kappa^2), \tag{28}$$

with the κ-independent terms

$$Y = -\frac{4g^2}{\Omega^2}\coth\frac{\Omega}{2T}, \quad W = \frac{4g^2}{\Omega^2} \tag{29}$$

and the terms linear in κ

$$A = -\Gamma\frac{Y}{2}, \quad B = \Gamma\frac{8g^2T}{\Omega^3} \tag{30}$$

$$C = -\Gamma\frac{2g^2}{\Omega^3}\frac{\Omega/T + 2\sinh\Omega/T}{\cosh\Omega/T}, \quad V = \Gamma\frac{4g^2}{\Omega^3}. \tag{31}$$