differences in z-direction is

$$V_I(q_{i,j}, q_{i+q,j+s}) = C\left(\frac{1}{d_{xy}} - \frac{(q_{i,j} - q_{i+q,j+s})^2}{2\,(d_{xy})^3} + ...\right) \tag{0.206}$$

which is basically the quadratic interaction from above, this lets us expect similar behavior and motivates the benchmarking of quadratic interaction.
The force acting between two particles will then be

$$\frac{\partial V_I(q_{i,j}, q_{i+q,j+s})}{\partial q_{i,j}} = -C\left(\frac{(q_{i,j} - q_{i+q,j+s})}{\left((qa_x)^2 + (sa_y)^2 + (q_{i,j} - q_{i+q,j+s})^2\right)^{3/2}}\right) \tag{0.207}$$

0.2.4 Quantum Description

We will try to describe our model as a two state system, each state living in a displaced harmonic oscillator. The hamiltonian of one lattice site then would be

$$H_S = P_0\varepsilon_0 + P_1\varepsilon_1 + \lambda(P_0 - P_1) \otimes (a^\dagger + a) + \Omega a^\dagger a \tag{0.208}$$

This hamiltonian is not diagonal in the eigen-energy basis of the harmonic oscillator which would make the transition to interaction picture difficult. Thats why we introduce the polaron transformation:

$$U_p = e^{\frac{\lambda}{\Omega}(P_0 - P_1)\otimes(a^\dagger - a)} \tag{0.209}$$

To transform H_S into the polaron picture, we need to know how the polaron transformation acts on $a^{(\dagger)}$:

$$U_p a = \sum_{k=0}^{\infty} \frac{\left(\frac{\lambda}{\Omega}(P_0 - P_1)\right)^k}{k!} \otimes (a^\dagger - a)^k a \tag{0.210}$$

$$= \sum_{k=0}^{\infty} \frac{\left(\frac{\lambda}{\Omega}(P_0 - P_1)\right)^k}{k!} \otimes \left(a(a^\dagger - a)^k - k(a^\dagger - a)^{k-1}\right) \tag{0.211}$$

$$= aU_p - \left(\frac{\lambda}{\Omega}(P_0 - P_1)\right) \sum_k \frac{\left(\frac{\lambda}{\Omega}(P_0 - P_1)\right)^{k-1} \cancel{k}(a^\dagger - a)^{k-1}}{\cancel{k}(k-1)!} \tag{0.212}$$

$$= aU_p - \left(\frac{\lambda}{\Omega}(P_0 - P_1)\right) U_p \tag{0.213}$$

Implying that

$$a_p = U_p a U_p^\dagger = a - \left(\frac{\lambda}{\Omega}(P_0 - P_1)\right) \quad \text{and} \quad a_p^\dagger = a^\dagger - \left(\frac{\lambda}{\Omega}(P_0 - P_1)\right) \tag{0.214}$$

The projectors transform trivially since they commute with every operator in the polaron transformation. For the transformed Hamiltonian we then get

$$\begin{aligned}
H_S^P = U_P H_S U_P^\dagger =& P_0\varepsilon_0 + P_1\varepsilon_1 + \lambda(P_0 - P_1) \otimes (U_p a^\dagger U_p^\dagger + U_p a U_p^\dagger) + \Omega U_p a^\dagger U_p^\dagger U_p a U_p^\dagger \\
=& P_0\varepsilon_0 + P_1\varepsilon_1 + \lambda(P_0 - P_1) \otimes \left(a - \left(\frac{\lambda}{\Omega}(P_0 - P_1)\right) + a^\dagger - \left(\frac{\lambda}{\Omega}(P_0 - P_1)\right)\right) \\
&+ \Omega \left(a^\dagger - \left(\frac{\lambda}{\Omega}(P_0 - P_1)\right)\right)\left(a - \left(\frac{\lambda}{\Omega}(P_0 - P_1)\right)\right) \\
=& P_0\varepsilon_0 + P_1\varepsilon_1 + \lambda(P_0 - P_1) \otimes (a^\dagger + a) - \frac{\lambda^2}{\Omega} - \frac{\lambda^2}{\Omega} \\
&+ \Omega a^\dagger a - \Omega\frac{\lambda}{\Omega}(P_0 - P_1) \otimes (a^\dagger + a) + \Omega\frac{\lambda^2}{\Omega^2} \\
=& P_0\varepsilon_0 + P_1\varepsilon_1 - \frac{\lambda^2}{\Omega} + \Omega a^\dagger a
\end{aligned}$$

Interaction with state transition

If we want to describe a transition from one well to another of the double well potential, we need to model transitions from state $|0\rangle$ to $|1\rangle$ (and the other way around), which means we need to consider jump operators like

$$\sigma^- = |0\rangle\langle 1| \qquad \text{and} \qquad \sigma^+ = (\sigma^-)^\dagger = |1\rangle\langle 0| \tag{0.215}$$

with (BCH)

$$\begin{aligned}
U_p\sigma^- U_p^\dagger =& \sigma^- + \left[\frac{\lambda}{\Omega}(P_0 - P_1) \otimes (a^\dagger - a), \sigma^-\right] \\
&+ \frac{1}{2!}\left[\frac{\lambda}{\Omega}(P_0 - P_1) \otimes (a^\dagger - a), \left[\frac{\lambda}{\Omega}(P_0 - P_1) \otimes (a^\dagger - a), \sigma^-\right]\right] \\
&+ \ldots \\
=& \sigma^- + \sigma^- \frac{2\lambda}{\Omega}(a^\dagger - a) + \sigma^- \frac{1}{2!}\left(\frac{2\lambda}{\Omega}(a^\dagger - a)\right)^2 + \ldots \\
=& \sigma^- e^{\frac{2\lambda}{\Omega}(a^\dagger - a)} \\
=& \sigma_p^-
\end{aligned}$$

The interaction Hamiltonian that we want to look at will be

$$H_I^p = A_I^p \otimes B_I = (\sigma_p^- + \sigma_p^+) \otimes \sum_k (h_k b_k + h_k^* b_k^\dagger) \tag{0.216}$$

Since we want to go into the interaction picture with respect to H_S^P and $H_B = \sum_k \omega_k b_k^\dagger b_k$, we need to know the time evolution of σ_p^-:

$$\boldsymbol{\sigma}_p^- = e^{iH_S^p t}\sigma_p^- e^{-iH_S^p t} = e^{i(P_0\varepsilon_0+P_1\varepsilon_1)t}\sigma^- e^{-i(P_0\varepsilon_0+P_1\varepsilon_1)t} e^{i(\Omega a^\dagger a)t} e^{\frac{2\lambda}{\Omega}(a^\dagger - a)} e^{-i(\Omega a^\dagger a)t} \tag{0.217}$$

Since $P_a^k = P_a$, we can rewrite

$$e^{iP_0\epsilon_0 t} = \sum_{k=0} \frac{(i\varepsilon_0 t)^k}{k!} P_0^k = 1 + \sum_{k=1} \frac{(i\varepsilon_0 t)^k}{k!} P_0 = 1 + (e^{i\varepsilon_0 t} - 1)P_0 \tag{0.218}$$

With that

$$e^{i(P_0\varepsilon_0)t}\sigma^- e^{-i(P_0\varepsilon_0)t} = \left[1 + (e^{i\varepsilon_0 t} - 1)P_0\right] \sigma^- \left[1 + (e^{-i\varepsilon_0 t} - 1)P_0\right] = \sigma^- e^{i\varepsilon_0 t} \tag{0.219}$$

For $e^{i(\Omega a^\dagger a)t} e^{\frac{2\lambda}{\Omega}(a^\dagger - a)} e^{-i(\Omega a^\dagger a)t}$ we can use that the time evolution is unitary and write

$$e^{i(\Omega a^\dagger a)t} e^{\frac{2\lambda}{\Omega}(a^\dagger - a)} e^{-i(\Omega a^\dagger a)t} = e^{\frac{2\lambda}{\Omega} e^{i(\Omega a^\dagger a)t}(a^\dagger - a)e^{-i(\Omega a^\dagger a)t}} \tag{0.220}$$

Which reduces the problem to calculating $e^{i(\Omega a^\dagger a)t} a^{(\dagger)} e^{-i(\Omega a^\dagger a)t}$. We do that by deriving a differential equation:

$$\frac{d}{dt}\tilde{a}(t) = \frac{d}{dt}\left(e^{i(\Omega a^\dagger a)t} a e^{-i(\Omega a^\dagger a)t}\right) = e^{i(\Omega a^\dagger a)t}\left[i\Omega a^\dagger a, a\right] e^{-i(\Omega a^\dagger a)t} \tag{0.221}$$

$$= -i\Omega\tilde{a}(t) \tag{0.222}$$

Which implies that $\tilde{a}(t) = Ce^{-i\Omega t}$, and with the initial condition that $\tilde{a}(0) = a$ we get

$$\tilde{a}(t) = e^{i(\Omega a^\dagger a)t} a e^{-i(\Omega a^\dagger a)t} = a e^{-i\Omega t} \tag{0.223}$$

That gives us in total

$$\boldsymbol{\sigma}_p^-(t) = \sigma^- e^{i(\varepsilon_0 - \varepsilon_1)t} \otimes e^{\frac{2\lambda}{\Omega}(a^\dagger e^{i\Omega t} - a e^{-i\Omega t})} \tag{0.224}$$

so that we can now express $\mathbf{A}_I^p(t) = \boldsymbol{\sigma}_p^-(t) + \boldsymbol{\sigma}_p^+(t)$. For deriving a Lindblad-Equation, we start at the Redfield-II equation that already has the degrees of freedom of the bath traced out:

$$\dot{\boldsymbol{\rho}}_S^p(t) = -\int_0^\infty \left[\boldsymbol{A}_I^p(t), \boldsymbol{A}_I^p(t-\tau)\boldsymbol{\rho}_S^p(t)\right] C(\tau)d\tau + h.c. \tag{0.225}$$

$$= -\int_0^\infty \left[\boldsymbol{\sigma}_p^-(t) + \boldsymbol{\sigma}_p^+(t), \boldsymbol{\sigma}_p^-(t-\tau) + \boldsymbol{\sigma}_p^+(t-\tau)\boldsymbol{\rho}_S^p(t)\right] C(\tau)d\tau + h.c. \tag{0.226}$$

If we want to do the secular approximation now, we need to consider the $e^{e^{\pm i\Omega t}}$ factors in $\boldsymbol{\sigma}_p^{\pm}(t)$ and one (or the only) way to do this is rewriting $\boldsymbol{\sigma}_p^{\pm}(t)$ as exponential series:

$$\boldsymbol{\sigma}_p^{-}(t) = \sum_{k,l} e^{-\frac{2\lambda^2}{\Omega^2}} \frac{\left(\frac{2\lambda}{\Omega}\right)^k \left(-\frac{2\lambda}{\Omega}\right)^l}{k!l!} e^{ik\Omega t}(a^\dagger)^k e^{-il\Omega t} a^l \otimes e^{i(\varepsilon_0-\varepsilon_1)t}\sigma^- \tag{0.227}$$

$$= \sum_{k,l} e^{-\frac{2\lambda^2}{\Omega^2}} \frac{\left(\frac{2\lambda}{\Omega}\right)^k \left(-\frac{2\lambda}{\Omega}\right)^l}{k!l!} (a^\dagger)^k a^l \otimes \sigma^- e^{i(\varepsilon_0-\varepsilon_1+(k-l)\Omega)t} \tag{0.228}$$

If we now look at combinations like $\boldsymbol{\sigma}_p^{-}(t)\boldsymbol{\sigma}_p^{-}(t-\tau)$, we see that (for every term)

$$\boldsymbol{\sigma}_p^{-}(t)\boldsymbol{\sigma}_p^{-}(t-\tau) \propto e^{i(2(\varepsilon_0-\varepsilon_1)-(k-l)\Omega-(m-n)\Omega)t} \cdot e^{-i((\varepsilon_0-\varepsilon_1)+(m-n)\Omega)\tau} \tag{0.229}$$

If now $2(\varepsilon_0-\varepsilon_1)$ is not an integer multiple of Ω, as we will assume in the following, terms like $\boldsymbol{\sigma}_p^{\pm}(t)\boldsymbol{\sigma}_p^{\pm}(t-\tau)\boldsymbol{\rho}_S^p(t)$ or $\boldsymbol{\sigma}_p^{\pm}(t-\tau)\boldsymbol{\rho}_S^p(t)\boldsymbol{\sigma}_p^{\pm}(t)$ will oscillate in t and are thus dropped in secular approximation. Therefore we are only interested in terms like:

$$\begin{aligned}\boldsymbol{\sigma}_p^{\pm}(t)\boldsymbol{\sigma}_p^{\mp}(t-\tau)\boldsymbol{\rho}_S^p(t) &= \sum_{klmn} D^{\mp}_{klmn} e^{\mp i(\varepsilon_0-\varepsilon_1)\tau} e^{i(k-l)\Omega t} e^{i(m-n)\Omega(t-\tau)} (a^\dagger)^k a^l (a^\dagger)^m a^n \sigma^+\sigma^- \boldsymbol{\rho}_S^p(t)\\ &\propto e^{i(\mp(\varepsilon_0-\varepsilon_1)-(m-n)\Omega)\tau} \cdot e^{i(k-l+m-n)t}\end{aligned}$$

$$\begin{aligned}\boldsymbol{\sigma}_p^{\pm}(t-\tau)\boldsymbol{\rho}_S^p(t)\boldsymbol{\sigma}_p^{\mp}(t) &= \sum_{klmn} D^{\mp}_{klmn} e^{\pm i(\varepsilon_0-\varepsilon_1)\tau} e^{i(k-l)\Omega(t-\tau)} e^{i(m-n)\Omega t} \sigma^- (a^\dagger)^k a^l \boldsymbol{\rho}_S^p(t) (a^\dagger)^m a^n \sigma^+\\ &\propto e^{i(\pm(\varepsilon_0-\varepsilon_1)-(k-l)\Omega)\tau} \cdot e^{i(k-l+m-n)t}\end{aligned}$$

The last exponential factor oscillating in t yields in secular approximation a delta distribution of the form $\delta_{k-l,n-m}$.
The property of the prefactor

$$D^{+}_{klmn} = e^{\frac{4\lambda^2}{\Omega^2}} \frac{\left(\frac{2\lambda}{\Omega}\right)^{k+n} \left(-\frac{2\lambda}{\Omega}\right)^{l+m}}{k!l!m!n!} = D^{-}_{mnkl} \tag{0.230}$$

lets us combine the terms $\boldsymbol{\sigma}_p^{\pm}(t)\boldsymbol{\sigma}_p^{\mp}(t-\tau)\boldsymbol{\rho}_S^p(t) + \boldsymbol{\sigma}_p^{\mp}(t-\tau)\boldsymbol{\rho}_S^p(t)\boldsymbol{\sigma}_p^{\pm}(t)$ to

$$\begin{aligned}\dot{\boldsymbol{\rho}}_S^p(t) = &-\int_0^\infty \sum_{klmn} D^{+}_{klmn} \left[\sigma^- \otimes (a^\dagger)^k a^l, \sigma^+ \otimes (a^\dagger)^m a^n \boldsymbol{\rho}_S^p\right] e^{i((\varepsilon_0-\varepsilon_1)-(m-n)\Omega)\tau} C(\tau)\delta_{k-l,n-m} d\tau\\ &-\int_0^\infty \sum_{klmn} D^{-}_{klmn} \left[\sigma^+ \otimes (a^\dagger)^k a^l, \sigma^- \otimes (a^\dagger)^m a^n \boldsymbol{\rho}_S^p\right] e^{i((\varepsilon_1-\varepsilon_0)-(m-n)\Omega)\tau} C(\tau)\delta_{k-l,n-m} d\tau\\ &+ h.c.\end{aligned}$$

The calculation of the Correlation function $C(\tau)$ will be written down later, if we express it through the spectral coupling density, we can write it as a fourier transform:

$$C(\tau) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \gamma(\omega) e^{-i\omega\tau} d\omega \tag{0.231}$$

Inserted in the equation above (and using $\Delta\varepsilon = \varepsilon_0 - \varepsilon_1$)

$$\begin{aligned}\dot{\boldsymbol{\rho}}_S^p(t) = &-\int_{-\infty}^{\infty}\int_0^{\infty}\sum_{klmn} D^+_{klmn}\left[..,..\right] e^{-i(\omega-\Delta\varepsilon+(m-n)\Omega)\tau}\frac{1}{2\pi}\gamma(\omega)\delta_{k-l,n-m} d\tau d\omega \\ &-\int_{-\infty}^{\infty}\int_0^{\infty}\sum_{klmn} D^-_{klmn}\left[..,..\right] e^{-i(\omega+\Delta\varepsilon+(m-n)\Omega)\tau}\frac{1}{2\pi}\gamma(\omega)\delta_{k-l,n-m} d\tau d\omega \\ &+ h.c.\end{aligned}$$

We can now use the **Sokhotskij-Plemelj theorem** to perform the $\int d\tau$- integration, leading to

$$\begin{aligned}\dot{\boldsymbol{\rho}}_S^p(t) = &-\int_{-\infty}^{\infty}\sum_{klmn} D^+_{klmn}\left[...\right]\gamma(\omega)\left(\frac{1}{2}\delta(\omega-(\Delta\varepsilon-(m-n)\Omega)) - \frac{i}{2\pi}\mathcal{P}\frac{1}{\omega-\Delta\varepsilon+(m-n)\Omega}\right)\delta_{k-l,n} \\ &-\int_{-\infty}^{\infty}\sum_{klmn} D^-_{klmn}\left[...\right]\gamma(\omega)\left(\frac{1}{2}\delta(\omega+(\Delta\varepsilon+(m-n)\Omega)) - \frac{i}{2\pi}\mathcal{P}\frac{1}{\omega+\Delta\varepsilon+(m-n)\Omega}\right)\delta_{k-l,n} \\ &+ h.c.\end{aligned}$$

The second term in the integrals results in the lambs shift which is small and which will be neglected in the following. We can use the δ-Distribution to perform the $\int d\omega$-integration, leading to our, for now, final result:

$$\begin{aligned}\dot{\boldsymbol{\rho}}_S^p(t) = &-\frac{1}{2}\sum_{klmn} D^+_{klmn}\gamma(\Delta\varepsilon-(m-n)\Omega)\left\{\left[\sigma^-\otimes(a^\dagger)^k a^l, \sigma^+\otimes(a^\dagger)^m a^n\boldsymbol{\rho}_S^p\right] + h.c.\right\}\delta_{k-l,n-m} \\ &-\frac{1}{2}\sum_{klmn} D^-_{klmn}\gamma(-\Delta\varepsilon-(m-n)\Omega)\left\{\left[\sigma^+\otimes(a^\dagger)^k a^l, \sigma^-\otimes(a^\dagger)^m a^n\boldsymbol{\rho}_S^p\right] + h.c.\right\}\delta_{k-l,n-m}\end{aligned}$$

This is still not in Lindblad form and sadly also won't be since we have different powers of creation and annihilation operators in the commutator. We could transform back to the Schrödinger picture now via

$$\dot{\rho}_S^p(t) = -i\left[H_S^p, \rho_S^p(t)\right] + e^{-iH_S^p t}\dot{\boldsymbol{\rho}}_S^p(t)e^{iH_S^p t} \tag{0.232}$$

The $\delta_{k-l,n-m}$ factor ensures that the $e^{i\Omega t}$-Terms that arise when we transform the $a^{(\dagger)}$ compensate so that we just get for the (not yet) Lindblad equation

$$\begin{aligned}
\dot{\rho}_S^p(t) =& -i\left[H_S^p, \rho_S^p(t)\right] \\
&- \frac{1}{2}\sum_{klmn} D^+_{klmn}\gamma(\Delta\varepsilon - (m-n)\Omega)\left\{\left[\sigma^- \otimes (a^\dagger)^k a^l, \sigma^+ \otimes (a^\dagger)^m a^n \rho_S^p\right] + h.c.\right\}\delta_{k-l,n-m} \\
&- \frac{1}{2}\sum_{klmn} D^-_{klmn}\gamma(-\Delta\varepsilon - (m-n)\Omega)\left\{\left[\sigma^+ \otimes (a^\dagger)^k a^l, \sigma^- \otimes (a^\dagger)^m a^n \rho_S^p\right] + h.c.\right\}\delta_{k-l,n-m}
\end{aligned}$$

From here i don't now how to calculate expectation values because of the powers of the creation and annihilation operators. But i tried anyway for the seemingly easiest case $\frac{d}{dt}\langle\sigma^-\rangle$: It seemed easier to transform back to the "normal" picture, since otherwise we would have had to calculate $[\sigma_p^\pm, (a^{(\dagger)})^k]$. Doing the transformation yields:

$$\begin{aligned}
\dot{\rho}_S(t) =& U_p^\dagger \dot{\rho}_S^p(t) U_p \\
=& -i\left[H_S, \rho_S(t)\right] \\
&- \frac{1}{2}\sum_{klmn} D^+_{klmn}\gamma(\Delta\varepsilon - (m-n)\Omega)\left\{\left[\sigma^-_{-p} \otimes (a^\dagger_{-p})^k a^l_{-p}, \sigma^+_{-p} \otimes (a^\dagger_{-p})^m a^n_{-p}\rho_S\right] + h.c.\right\}\delta_{k-l,n-m} \\
&- \frac{1}{2}\sum_{klmn} D^-_{klmn}\gamma(-\Delta\varepsilon - (m-n)\Omega)\left\{\left[\sigma^+_{-p} \otimes (a^\dagger_{-p})^k a^l_{-p}, \sigma^-_{-p} \otimes (a^\dagger_{-p})^m a^n_{-p}\rho_S\right] + h.c.\right\}\delta_{k-l,n-m}
\end{aligned}$$

With $_{-p}$ denoting the polaron transformation with $\lambda' = -\lambda$ yielding

$$\sigma^\pm_{-p} = \sigma^\pm e^{\pm\frac{2\lambda}{\Omega}(a^\dagger - a)} \qquad \text{and} \qquad a^{(\dagger)}_{-p} = a^{(\dagger)} + \frac{\lambda}{\Omega}(P_0 - P_1) \tag{0.233}$$

The commutator of $[(a^{(\dagger)}_{-p})^k, \sigma^-]$ is zero:

$$\begin{aligned}
(a^{(\dagger)}_{-p})^k\sigma^- =& (a^{(\dagger)} + \frac{\lambda}{\Omega}(P_0 - P_1))^k\sigma^- = \sum_i \binom{k}{i}(a^{(\dagger)})^{k-i}\left(\frac{\lambda}{\Omega}\right)^i (P_0 - P_1)^i\sigma^- \\
=& \sum_i \binom{k}{i}(a^{(\dagger)})^{k-i}\left(\frac{\lambda}{\Omega}\right)^i \begin{cases} \mathbf{1}\sigma^- & \text{i even} \\ (P_0 - P_1)\sigma^- & \text{i uneven} \end{cases} \\
=& \sigma^- \sum_i \binom{k}{i}(a^{(\dagger)})^{k-i}\left(\frac{\lambda}{\Omega}\right)^i (P_0 - P_1)^i = \sigma^-(a^{(\dagger)}_{-p})^k
\end{aligned}$$

Now we are ready to "compute" $\frac{d}{dt}\langle\sigma^-\rangle$ via $\frac{d}{dt}\langle\sigma^-\rangle = \mathrm{tr}\{\sigma^-\dot{\rho}_S\}$. We split the calculation into three terms, each representing one line of the equation for $\dot{\rho}_S$:

$$\begin{aligned}
(1) =& -i\ \mathrm{tr}\left\{\sigma^-\left[H_S,\rho_S\right]\right\}\\
=& -i\ \mathrm{tr}\left\{\sigma^- P_0\varepsilon_0\rho_S + \sigma^- P_1\varepsilon_1\rho_S + \lambda(P_0-P_1)\otimes(a^\dagger+a)\rho_S + \sigma^-\Omega a^\dagger a\rho_S\right\}\\
&-i\ \mathrm{tr}\left\{\sigma^-\rho_S\varepsilon_0 P_0 - \sigma^-\rho_S\varepsilon_1 P_1 - \sigma^-\rho_S\lambda(P_0-P_1)\otimes(a^\dagger+a) - \sigma^-\rho_S\Omega a^\dagger a\right\}\\
=& -i\ \mathrm{tr}\left\{(\varepsilon_1-\varepsilon_0)\sigma^-\rho_S - 2\lambda\sigma^-\otimes(a^\dagger+a)\rho_S\right\}\\
=&\ i\Delta\varepsilon\langle\sigma^-\rangle + 2i\lambda\langle\sigma^-\rangle\sqrt{2\Omega}\langle x\rangle
\end{aligned}$$

Here i already am suspicious that this differential equation is complex? The next terms only become worse:

$$\begin{aligned}
(2) =& -\frac{1}{2}\sum_{klmn} D^+_{klmn}\gamma(...)\mathrm{tr}\left\{\sigma^-\left[\sigma^-_{-p}\otimes(a^\dagger_{-p})^k a^l_{-p}, \sigma^+_{-p}\otimes(a^\dagger_{-p})^m a^n_{-p}\rho_S\right]\right\}\delta_{k-l,n-m}\\
&-\frac{1}{2}\sum_{klmn} D^+_{klmn}\gamma(...)\mathrm{tr}\left\{\sigma^-\left[\rho_S\sigma^-_{-p}\otimes(a^\dagger_{-p})^n a^m_{-p}, \sigma^+_{-p}\otimes(a^\dagger_{-p})^l a^k_{-p}\right]\right\}\delta_{k-l,n-m}
\end{aligned}$$

Since $\sigma^-\sigma^- = 0$ and we can freely swap cyclic and commute, actually only one term survives and we get

$$(2) = -\frac{1}{2}\sum_{klmn} D^+_{klmn}\gamma(...)\mathrm{tr}\left\{\sigma^- e^{-\frac{2\lambda}{\Omega}(a^\dagger-a)}(a^\dagger_{-p})^n a^m_{-p}(a^\dagger_{-p})^l a^k_{-p}\right\} \tag{0.234}$$

Yeah i don't now what to do after here.

Getting to Lindblad-Form Starting from the Master equation in polaron-schrödinger picture, we consider the term

$$D^+_{klmn}\gamma^+_{(m-n)}\left\{\left[\sigma^-(a^\dagger)^k a^l, \sigma^+(a^\dagger)^m a^n\rho^p_S\right] + \left[\rho^p_S\sigma^-(a^\dagger)^n a^m, \sigma^+(a^\dagger)^l a^k\right]\right\}\delta_{k-l,n-m} \tag{0.235}$$

using $\gamma^+_{m-n} = \gamma(\Delta\varepsilon - (m-n)\Omega)$. We make the replacements $l = m, k = n$ in the second term, which yields

$$\left\{\gamma^+_{(m-n)}D^+_{klmn}\left[\sigma^-(a^\dagger)^k a^l, \sigma^+(a^\dagger)^m a^n\rho^p_S\right] + \gamma^+_{(l-k)}D^+_{nmlk}\left[\rho^p_S\sigma^-(a^\dagger)^k a^l, \sigma^+(a^\dagger)^m a^n\right]\right\}\delta_{k-l,n-m}$$

Note that $D^+_{klmn} = D^+_{nmlk}$ and $\gamma^+_{(m-n)}\delta_{k-l,n-m} = \gamma^+_{(l-k)}\delta_{k-l,n-m}$, so that we get

$$\begin{aligned}
= \gamma^+_{(m-n)}D^+_{klmn}\quad & \{\sigma^-(a^\dagger)^k a^l\sigma^+(a^\dagger)^m a^n\rho^p_S - \sigma^+(a^\dagger)^m a^n\rho^p_S\sigma^-(a^\dagger)^k a^l && (0.236)\\
& + \rho^p_S\sigma^-(a^\dagger)^k a^l\sigma^+(a^\dagger)^m a^n - \sigma^+(a^\dagger)^m a^n\rho^p_S\sigma^-(a^\dagger)^k a^l\}\delta_{k-l,n-m} && (0.237)\\
= -\gamma^+_{(m-n)}D^+_{klmn}\quad & \left\{2\sigma^+(a^\dagger)^m a^n\rho^p_S\sigma^-(a^\dagger)^k a^l - \left\{\sigma^-\sigma^+(a^\dagger)^k a^l(a^\dagger)^m a^n, \rho^p_S\right\}\right\}\delta_{k-l,n-m} && (0.238)
\end{aligned}$$

Which looks a bit more Lindblad but still isn't. To get to a Lindblad form we rewrite the sum

$$\sum_{klmn} \gamma^{+}_{(m-n)} D^{+}_{klmn} \left\{ 2\sigma^{+}(a^{\dagger})^{m} a^{n} \rho^{p}_{S} \sigma^{-}(a^{\dagger})^{k} a^{l} - \left\{ \sigma^{-}\sigma^{+}(a^{\dagger})^{k} a^{l} (a^{\dagger})^{m} a^{n}, \rho^{p}_{S} \right\} \right\} \delta_{k-l,n-m} \quad (0.239)$$

to sum over $q = l-k$ and $r = m-n$ (if i am not mistaken $\sum_{k=0,l=0}^{\infty} A^k B^l = \sum_{q=0}^{\infty} \sum_{k=0}^{\infty} A^k B^{k+q}$):

$$\begin{aligned}
&= \sum_{q=0,r=0}^{\infty} \sum_{kn} \gamma^{+}_{(r)} D^{+}_{k,k+q} D^{+}_{n,n+r} \left\{ 2\sigma^{+}(a^{\dagger})^{n+r} a^{n} \rho^{p}_{S} \sigma^{-}(a^{\dagger})^{k} a^{k+q} - \left\{ \sigma^{-}\sigma^{+}(a^{\dagger})^{k} a^{k+q} (a^{\dagger})^{n+r} a^{n}, \rho^{p}_{S} \right\} \right\} \delta_{r,q} \\
&= \sum_{q} \Bigg\{ 2 \left(\sqrt{\gamma^{+}_{q}} \sum_{n} D^{+}_{n,n+q} \sigma^{+} (a^{\dagger})^{n+q} a^{n} \right) \rho^{p}_{S} \left(\sqrt{\gamma^{+}_{q}} \sum_{k} D^{+}_{k,k+q} \sigma^{-} (a^{\dagger})^{k} a^{k+q} \right) \\
&\quad - \left\{ \left(\sqrt{\gamma^{+}_{q}} \sum_{k} D^{+}_{k,k+q} \sigma^{-} (a^{\dagger})^{k} a^{k+q} \right) \left(\sqrt{\gamma^{+}_{q}} \sum_{n} D^{+}_{n,n+q} \sigma^{+} (a^{\dagger})^{n+q} a^{n} \right), \rho^{p}_{S} \right\} \Bigg\}
\end{aligned}$$

With

$$D^{+}_{k,k+q} = e^{\frac{2\lambda^2}{\Omega^2}} \frac{\left(\frac{2\lambda}{\Omega}\right)^{k} \left(-\frac{2\lambda}{\Omega}\right)^{k+q}}{k!(k+q)!} \quad (0.240)$$

Since we can obviously rename $n \to k$ and $\left(\sqrt{\gamma^{+}_{q}} \sum_{k} D^{+}_{k,k+q} \sigma^{+} (a^{\dagger})^{k+q} a^{k}\right)^{\dagger} = \left(\sqrt{\gamma^{+}_{q}} \sum_{k} D^{+}_{k,k+q} \sigma^{-} (a^{\dagger})^{k} a^{k+q}\right)$, we have achieved Lindblad form with the jump operator:

$$L^{+}_{q} = \sqrt{\gamma^{+}_{q}} \sum_{k} D^{+}_{k,k+q} \sigma^{+} (a^{\dagger})^{k+q} a^{k} \quad (0.241)$$

For the term with the $\gamma^{-}_{q} = \gamma(-\Delta\varepsilon - q\Omega))$ prefactor we can do the same calculation and arrive at the jump operator

$$L^{-}_{q} = \sqrt{\gamma^{-}_{q}} \sum_{k} D^{-}_{k,k+q} \sigma^{-} (a^{\dagger})^{k+q} a^{k} \quad (0.242)$$

Which lets us write down the Lindblad equation in polaron picture:

$$\begin{aligned}
\dot{\rho}^{p}_{S}(t) = &- i \left[H^{p}_{S}, \rho^{p}_{S}(t) \right] \\
&+ \sum_{q} \left(L^{+}_{q} \rho^{p}_{S} \left(L^{+}_{q}\right)^{\dagger} - \frac{1}{2} \left\{ \left(L^{+}_{q}\right)^{\dagger} L^{+}_{q}, \rho^{p}_{S} \right\} \right) \\
&+ \sum_{q} \left(L^{-}_{q} \rho^{p}_{S} \left(L^{-}_{q}\right)^{\dagger} - \frac{1}{2} \left\{ \left(L^{-}_{q}\right)^{\dagger} L^{-}_{q}, \rho^{p}_{S} \right\} \right)
\end{aligned}$$

To pursue the idea that we can factorize the two-level expectation values and the harmonic-oscillator expectation values, we transform back into the "normal" picture to calculate $\frac{d}{dt}\langle\sigma^{-}\rangle$.

We need to know how the jump operators transform:

$$U_p^\dagger L_q^+ U_p = \sqrt{\gamma_q^+} \sum_k D_{k,k+q}^+ \sigma_{-p}^+ (a_{-p}^\dagger)^{k+q} a_{-p}^k \tag{0.243}$$

$$= \sqrt{\gamma_q^+} \sum_k D_{k,k+q}^+ \sigma^+ e^{\frac{2\lambda}{\Omega}\left(a^\dagger - a\right)} \left(a^\dagger + \frac{\lambda}{\Omega}\sigma^z\right)^{k+q} \left(a + \frac{\lambda}{\Omega}\sigma^z\right)^k \tag{0.244}$$

It is straightforward to commute σ^+ and a_p:

$$\sigma^+ \left(a + \frac{\lambda}{\Omega}\sigma^z\right)^k = \sigma^+ \left(a + \frac{\lambda}{\Omega}\sigma^z\right) \left(a + \frac{\lambda}{\Omega}\sigma^z\right)^{k-1} = \left(a + \frac{\lambda}{\Omega}\right) \sigma^+ \left(a + \frac{\lambda}{\Omega}\sigma^z\right)^{k-1} \tag{0.245}$$

$$= \left(a + \frac{\lambda}{\Omega}\right)^k \sigma^+ \tag{0.246}$$

which leads to

$$U_p^\dagger L_q^+ U_p = \sqrt{\gamma_q^+} \sum_k D_{k,k+q}^+ e^{\frac{2\lambda}{\Omega}\left(a^\dagger - a\right)} \left(a^\dagger + \frac{\lambda}{\Omega}\right)^{k+q} \left(a + \frac{\lambda}{\Omega}\right)^k \otimes \sigma^+ \tag{0.247}$$

$$= \mathcal{L}_q^+ \otimes \sigma^+ \tag{0.248}$$

And $\mathcal{L}_q^+$ acting only on the bosonic modes. So in the normal picture the Lindblad equation has the form

$$\dot{\rho}_S(t) = -\, i \left[H_S, \rho_S(t)\right] \tag{0.249}$$

$$+ \sum_q \left(\mathcal{L}_q^+ \otimes \sigma^+ \rho_S \left(\left(\mathcal{L}_q^+\right)^\dagger \otimes \sigma^- \right) - \frac{1}{2} \left\{ \left(\left(\mathcal{L}_q^+\right)^\dagger \otimes \sigma^- \right) \mathcal{L}_q^+ \otimes \sigma^+, \rho_S \right\} \right) \tag{0.250}$$

$$+ \sum_q \left(\mathcal{L}_q^- \otimes \sigma^- \rho_S \left(\left(\mathcal{L}_q^-\right)^\dagger \otimes \sigma^+ \right) - \frac{1}{2} \left\{ \left(\left(\mathcal{L}_q^-\right)^\dagger \otimes \sigma^+ \right) \mathcal{L}_q^- \otimes \sigma^-, \rho_S \right\} \right) \tag{0.251}$$

Interaction with only creation and annihilation operator

Looking at the Interaction (B as before)

$$H_I = (a^\dagger + a) \otimes B_I \qquad \Rightarrow \qquad \boldsymbol{H}_I^P(t) = (\boldsymbol{a}_p^\dagger + \boldsymbol{a}_p) \otimes \boldsymbol{B}_I \tag{0.252}$$

With

$$\boldsymbol{a}_p^{(\dagger)} = e^{iH_S^p t} a_p^{(\dagger)} e^{-iH_S^p t} = a^{(\dagger)} e^{(-)-i\Omega t} - \frac{\lambda}{\Omega}(P_0 - P_1) \tag{0.253}$$

Which gives us

$$\boldsymbol{H}_I^P(t) = \left(a^\dagger e^{i\Omega t} + a e^{-i\Omega t} - \frac{2\lambda}{\Omega}(P_0 - P_1)\right) \otimes \boldsymbol{B}_I \tag{0.254}$$

Since we use the same bath as before, we can again start at the Redfield-II equation:

$$\begin{aligned}
\dot{\boldsymbol{\rho}}_S^p(t) &= -\int_0^\infty \left[\boldsymbol{A}_I^p(t), \boldsymbol{A}_I^p(t-\tau)\boldsymbol{\rho}_S^p(t)\right] C(\tau) d\tau + h.c. \\
&= -\int_0^\infty \left[\boldsymbol{a}_p^\dagger(t) + \boldsymbol{a}_p(t), (\boldsymbol{a}_p^\dagger(t-\tau) + \boldsymbol{a}_p(t-\tau))\boldsymbol{\rho}_S^p(t)\right] C(\tau) d\tau + h.c. \\
&= -\int_0^\infty \left[a^\dagger e^{i\Omega t} + a e^{-i\Omega t} - \frac{2\lambda}{\Omega}(P_0 - P_1), \left(a^\dagger e^{i\Omega(t-\tau)} + a e^{-i\Omega(t-\tau)} - \frac{2\lambda}{\Omega}(P_0 - P_1)\right)\boldsymbol{\rho}_S^p(t)\right] C(\tau) d\tau
\end{aligned}$$

In secular approximation only terms with mixed $a, a^\dagger$ or none at all survive, leaving us with

$$\begin{aligned}
\dot{\boldsymbol{\rho}}_S^p(t) = -\int_0^\infty &\left\{\left[a^\dagger, a\boldsymbol{\rho}_S^p(t)\right] e^{i\Omega\tau} + \left[a, a^\dagger\boldsymbol{\rho}_S^p(t)\right] e^{-i\Omega\tau} + \frac{4\lambda^2}{\Omega^2}\left[(P_0 - P_1), (P_0 - P_1)\boldsymbol{\rho}_S^p(t)\right]\right\} C(\tau) d\tau \\
&+ h.c.
\end{aligned}$$

The first two terms are known from the calculation for the harmonic oscillator, which leaves us to deal with the last term.

$$\begin{aligned}
&-\int_0^\infty \left\{\frac{4\lambda^2}{\Omega^2}\left[(P_0 - P_1), (P_0 - P_1)\boldsymbol{\rho}_S^p(t)\right]\right\} C(\tau) d\tau + h.c \\
&= -\int_{-\infty}^\infty \int_0^\infty \left\{\frac{4\lambda^2}{\Omega^2}\left[(P_0 - P_1), (P_0 - P_1)\boldsymbol{\rho}_S^p(t)\right]\right\} \frac{1}{2\pi}\gamma(\omega) e^{-i\omega\tau} d\tau d\omega + h.c \\
&= -\int_{-\infty}^\infty \left\{\frac{4\lambda^2}{\Omega^2}\left[(P_0 - P_1), (P_0 - P_1)\boldsymbol{\rho}_S^p(t)\right]\right\} \gamma(\omega) \left\{\frac{1}{2}\delta(\omega) - \frac{i}{2\pi}\mathcal{P}\frac{1}{\omega}\right\} d\omega + h.c \\
&= -\frac{1}{2}\gamma(0)\frac{4\lambda^2}{\Omega^2}\left\{\left[(P_0 - P_1), (P_0 - P_1)\boldsymbol{\rho}_S^p(t)\right] + \left[\boldsymbol{\rho}_S^p(t)(P_0 - P_1), (P_0 - P_1)\right]\right\} \\
&\quad - \frac{i}{2\pi}\mathcal{P}\frac{4\lambda^2}{\Omega^2}\int_{-\infty}^\infty \frac{\gamma(\omega)}{\omega}\left\{\left[(P_0 - P_1), (P_0 - P_1)\boldsymbol{\rho}_S^p(t)\right] - \left[\boldsymbol{\rho}_S^p(t)(P_0 - P_1), (P_0 - P_1)\right]\right\} \\
&= +\frac{4\lambda^2}{\Omega^2}\gamma(0)\left[(P_0 - P_1)\boldsymbol{\rho}_S^p(t)(P_0 - P_1) - \boldsymbol{\rho}_S^p(t)\right] \\
&\quad - \frac{i}{2\pi}\mathcal{P}\frac{4\lambda^2}{\Omega^2}\int_{-\infty}^\infty \frac{\gamma(\omega)}{\omega}\left[(P_0 - P_1)^2, \boldsymbol{\rho}_S^p(t)\right] \qquad \text{This term is zero since } (P_0 - P_1)^2 = 1
\end{aligned}$$

When transforming to the Schrödinger picture, this new term also transforms trivially as the projection operators do not transform at all, which leaves us with

$$\rho_S^p(t) = -\, i \left[\varepsilon_0 P_0 + \varepsilon_1 P_1 + (\Omega + \Delta\Omega) a^\dagger a, \rho_S^p(t)\right] \tag{0.255}$$
$$+ \Gamma(\Omega) \left[1 + n_B(\Omega)\right] \left[a \rho_S^p(t) a^\dagger - \frac{1}{2} \left\{a^\dagger a, \rho_S^p(t)\right\}\right] \tag{0.256}$$
$$+ \Gamma(\Omega) n_B(\Omega) \left[a^\dagger \rho_S^p(t) a - \frac{1}{2} \left\{a a^\dagger, \rho_S^p(t)\right\}\right] \tag{0.257}$$
$$+ \frac{4\lambda^2}{\Omega^2} \Gamma(0) n_B(0) \left[(P_0 - P_1) \rho_S^p(t) (P_0 - P_1) - \rho_S^p(t)\right] \tag{0.258}$$

Now we can derive differential equations for the operator mean values. For a general operator C what actually should be true is

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle C\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{tr}\left\{C\rho_S\right\} = \mathrm{tr}\left\{C\frac{\mathrm{d}}{\mathrm{d}t}\rho_S\right\} = \mathrm{tr}\left\{C\frac{\mathrm{d}}{\mathrm{d}t}(U_p^\dagger \rho_S^p U_p)\right\} = \mathrm{tr}\left\{U_p C U_p^\dagger \frac{\mathrm{d}}{\mathrm{d}t}\rho_S^p\right\} \tag{0.259}$$
$$= \mathrm{tr}\left\{C_p \frac{\mathrm{d}}{\mathrm{d}t}\rho_S^p\right\} = \frac{\mathrm{d}}{\mathrm{d}t}\langle C_p\rangle \tag{0.260}$$

So it should not matter in which picture we calculate the differential equation. For some reason i get different results, probably a error, but I will present both ways here and hopefully recover the error in the process.

Calculation in polaron picture:

We start by calculating $\frac{\mathrm{d}}{\mathrm{d}t}\langle a_p\rangle$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle a_p\rangle = \mathrm{tr}\left\{\left(a - 1 \otimes \frac{\lambda}{\Omega}(P_0 - P_1)\right)\dot{\rho}_S^p\right\} = \mathrm{tr}\left\{a\dot{\rho}_S^p\right\} - \mathrm{tr}\left\{1 \otimes \frac{\lambda}{\Omega}(P_0 - P_1)\dot{\rho}_S^p\right\} \tag{0.261}$$

For a lindblad-equation, if an operator commutes with a certain jump operator $\left[L_k^{(\dagger)}, a\right] = 0$, the trace operation over the corresponding dissipator term will be zero since:

$$\mathrm{tr}\left\{a\left(L_k \rho_S L_k^\dagger - \frac{1}{2}\left\{L_k^\dagger L, \rho_S\right\}\right)\right\} = \mathrm{tr}\left\{a L_k \rho_S L_k^\dagger - \frac{1}{2} a L_k^\dagger L \rho_S - \frac{1}{2} a \rho_S L_k^\dagger L\right\} \tag{0.262}$$
$$= \mathrm{tr}\left\{a L_k^\dagger L \rho_S - \frac{1}{2} a L_k^\dagger L \rho_S - \frac{1}{2} a L_k^\dagger L \rho_S\right\} = 0 \tag{0.263}$$

The same applies for parts of system hamiltonian that the operator commutes with $[H_S^0, a] = 0$ with $H_S = H_S^0 + H_S^1$ since

$$\begin{aligned}\mathrm{tr}\left\{a\left[H_S^0 + H_S^1, \rho_S\right]\right\} &= \mathrm{tr}\left\{a\left[H_S^0, \rho_S\right]\right\} + \mathrm{tr}\left\{a\left[H_S^1, \rho_S\right]\right\} \\ &= \mathrm{tr}\left\{a H_S^0 \rho_S - a \rho_S H_S^0\right\} + \mathrm{tr}\left\{a\left[H_S^1, \rho_S\right]\right\} \\ &= \mathrm{tr}\left\{a H_S^0 \rho_S - a H_S^0 \rho_S\right\} + \mathrm{tr}\left\{a\left[H_S^1, \rho_S\right]\right\} = \mathrm{tr}\left\{a\left[H_S^1, \rho_S\right]\right\}\end{aligned}$$

Which means we only have to look after the not-commuting terms when performing the trace, meaning that $\mathrm{tr}\left\{a\dot{\rho}_S^p\right\}$ is basically calculated by the exact same steps as in the harmonic oscillator case, but we have to be careful when rewriting the trace as expectation value:

$$\begin{aligned}\mathrm{tr}\left\{a\dot{\rho}_S^p\right\} &= \left[-i\Omega - \frac{\Gamma(\Omega)}{2}\right]\mathrm{tr}\left\{a\rho_S^p\right\} = \left[-i\Omega - \frac{\Gamma(\Omega)}{2}\right]\mathrm{tr}\left\{\left(a_p + \frac{\lambda}{\Omega}(P_0 - P_1)\right)\rho_S^p\right\} \\ &= \left[-i\Omega - \frac{\Gamma(\Omega)}{2}\right]\left(\langle a_p\rangle + \frac{\lambda}{\Omega}\langle P_0 - P_1\rangle\right)\end{aligned}$$

In the second term, $\mathrm{tr}\left\{1 \otimes \frac{\lambda}{\Omega}(P_0 - P_1)\dot{\rho}_S^p\right\}$, the operator commutes with everything, so the trace operation yields just zero leaving us with:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle a_p\rangle = \left[-i\Omega - \frac{\Gamma(\Omega)}{2}\right]\left(\langle a_p\rangle + \frac{\lambda}{\Omega}\langle P_0 - P_1\rangle\right) \tag{0.264}$$

Complex conjugating yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle a_p^\dagger\rangle = \left[i\Omega - \frac{\Gamma(\Omega)}{2}\right]\left(\langle a_p^\dagger\rangle + \frac{\lambda}{\Omega}\langle P_0 - P_1\rangle\right) \tag{0.265}$$

Which lets us calculate a differential equation for the expectation value of x:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\left\langle\frac{1}{\sqrt{2\Omega}}(a_p^\dagger + a_p)\right\rangle = \frac{1}{\sqrt{2\Omega}}\left(\frac{\mathrm{d}}{\mathrm{d}t}\langle a_p^\dagger\rangle + \frac{\mathrm{d}}{\mathrm{d}t}\langle a_p\rangle\right) \tag{0.266}$$

$$= i\sqrt{\frac{\Omega}{2}}\left(\langle a_p^\dagger\rangle - \langle a_p\rangle\right) - \frac{\Gamma(\Omega)}{2\sqrt{2\Omega}}\left(\langle a_p^\dagger\rangle + \langle a_p\rangle + \frac{2\lambda}{\Omega}\langle P_0 - P_1\rangle\right) \tag{0.267}$$

$$= \langle p\rangle - \frac{\Gamma(\Omega)}{2}\left(\langle x\rangle + \frac{2\lambda}{\sqrt{2\Omega^3}}\langle P_0 - P_1\rangle\right) \tag{0.268}$$

Which only differs from the differential equation for the harmonic oscillator from the constant term that depends on whether we are in state 0 or 1. This seems logical considering that we looked at a harmonic potential that was imposed with a linear term that depended on the state.

For the differential equation of $\langle p\rangle$ we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\left\langle i\sqrt{\frac{\Omega}{2}}(a_p^\dagger - a_p)\right\rangle = i\sqrt{\frac{\Omega}{2}}\left(\frac{\mathrm{d}}{\mathrm{d}t}\langle a_p^\dagger\rangle - \frac{\mathrm{d}}{\mathrm{d}t}\langle a_p\rangle\right) \tag{0.269}$$

$$= i\sqrt{\frac{\Omega}{2}}i\Omega\left(\langle a_p^\dagger\rangle + \langle a_p\rangle\right) - \frac{\Gamma(\Omega)}{2}\sqrt{\frac{2}{\Omega}}\left(\langle a_p^\dagger\rangle - \langle a_p\rangle\right) + i\sqrt{\frac{\Omega}{2}}(2i\lambda)\langle P_0 - P_1\rangle \tag{0.270}$$

$$= -\Omega^2\langle x\rangle - \frac{\Gamma(\Omega)}{2}\langle p\rangle - \sqrt{2\Omega}\lambda\langle P_0 - P_1\rangle \tag{0.271}$$

TODO: How to get to a real Langevin equation from here or from the Lindblad equation?

Transitions induced by intra system

We now look at a lattice of interacting bosons which can each be in state $|0\rangle$ or $|1\rangle$. Every site is now coupled to its own bath of harmonic oscillators (since I think this yields the same calculation as for the one-site case and probably doesn't make a difference anyway). The system hamiltonian without site-to-site interaction will be

$$H_S^0 = \sum_j H_S^j = \sum_j \left[P_0^j\varepsilon_0 + P_1^j\varepsilon_1 + \lambda(P_0^j - P_1^j) \otimes ((a^j)^\dagger + a^j) + \Omega(a^j)^\dagger a^j\right] \tag{0.272}$$

And the total environment Hamiltonian:

$$H_B = \sum_j H_B^j \qquad \text{with } H_B \text{ as usual} \tag{0.273}$$

The transitions between the states are now not induced by the bath, but by the intra system interaction between the sites. To ensure that our hamiltonian has a lower spectral bound, we write the interaction into the $a^\dagger a$- Term:

$$H_S = \sum_j \left[... + \Omega \left((a^j)^\dagger + \frac{\xi}{\Omega} \sum_{i \in NN(j)} \left(\alpha^i \otimes \sigma_j^+\right) \right) \left(a^j + \frac{\xi}{\Omega} \sum_{i \in NN(j)} \left((\alpha^i)^\dagger \otimes \sigma_j^-\right) \right) \right] \tag{0.274}$$

With some operator α^i that acts on (the state Hilbert space of) site i and somehow makes the transition likelier if the neighboring site is in the opposite state.

If we expand this and neglect the term quadratic in $\frac{\xi}{\Omega}$ (only valid if it is small, so we assume small site to site interaction here), we get a representation of the form

$$H_S = H_S^0 + H_S^1 = \sum_j H_S^j + \sum_{ij} H_S^{ij} = \sum_j H_S^j + \sum_{\langle i,j \rangle} \left((a^j)^\dagger + a^j\right) \otimes \left(\alpha^i \otimes \sigma_j^+ + (\alpha^i)^\dagger \otimes \sigma_j^-\right) \tag{0.275}$$

I don't know whether this is a useful or sensible hamiltonian...

We could probably also just introduce for the Interaction a quadratic Term like

$$\left(1 + \xi \sum_{\langle i,j \rangle} \left(\alpha^i \otimes \sigma_j^+\right)\right) \left(1 + \xi \sum_{\langle i,j \rangle} \left((\alpha^i)^\dagger \otimes \sigma_j^-\right)\right) \tag{0.276}$$

Which would also ensure positivity and yield

$$H_S^1 = \xi \sum_{\langle i,j \rangle} \left(\alpha^i \otimes \sigma_j^+ + (\alpha^i)^\dagger \otimes \sigma_j^-\right) \qquad \text{(first order in } \xi \text{ neglecting constant terms)} \tag{0.277}$$

We could now go into interaction picture with respect to $H_S^0+H_B$, but then we would transform H_S^1 and get the exponential terms again. So I think the play here would be to go into interaction picture with respect to $H_S = H_S^0 + H_S^1 + H_B$?
If we now did the usual polaron transformation as before, the new H_S^p would contain e^a-Terms, which we want to avoid, since we then would have to deal with transformations like $e^{ie^a t} a e^{-ie^a} t$ and i can imagine this being very difficult. So we could either do no polaron transformation at all or a different one. I guess if we wrote the system hamiltonian as

$$H_S = \sum_j \Omega \left((a^j)^\dagger + \frac{\xi}{\Omega} \sum_{i \in NN(j)} \left(\alpha^i \otimes \sigma_j^+ \right) + \frac{\lambda}{\Omega} (P_0^j - P_1^j) \right) \cdot \left(a^j + \frac{\xi}{\Omega} \sum_{i \in NN(j)} \left((\alpha^i)^\dagger \otimes \sigma_j^- \right) + \frac{\lambda}{\Omega} (P_0^j - P_1^j) \right)$$

and neglected terms with $\frac{\lambda\xi}{\Omega}$, we would end up with our now defined Hamiltonian and then could try to define the coupling operator S as:

$$S_j = \frac{\xi}{\Omega} \sum_{i \in NN(j)} \left(\alpha^i \otimes \sigma_j^+ \right) + \frac{\lambda}{\Omega} (P_0^j - P_1^j) \tag{0.278}$$

and then try to do a Polaron transformation with

$$U_p = e^{\sum_j S_j} \tag{0.279}$$

I don't know, it might be possible to get a simple H_S^P with that? But seems difficult for now, it seems easier to just transform $e^{i(H_S^0+H_S^1)t} a_j e^{-i(H_S^0+H_S^1)t}$. What is $[H_S^0, H_S^1]$, it is sadly not just 0, right? Otherwise the transformation of a would be easy: $e^{iH_S^0 t} a e^{-iH_S^0 t}$. This is probably not a reasonable model...

Weak Coupling between $\hat{x}$ and σ^z

Another Idea would be to split the System Hamiltonian into:

$$\begin{aligned} H_S &= H_S^0 + H_S^1 \qquad \text{with} \\ H_S^0 &= \varepsilon + \Omega a^\dagger a \\ H_S^1 &= \lambda \sigma^z \otimes (a^\dagger + a) \qquad\qquad (\sigma^z = P_0 - P_1) \end{aligned}$$

And now going into Interaction picture with respect to $H_S^0 + H_B$ (H_B as usual), but I think this requires H_S^1 to be weak (with respect to H_S^0) somewhere along the way. It is questionable whether this is a reasonable assumption, since it would mean that (the first) excited states of the oscillator have larger energy than the "barrier" induced by H_S^1 and so the first excited state already lives in such high energy states that it differs strongly from the actual excited state in the double well potential. Anyway, we investigate if it at least yields some interesting dynamics.

We now allow the bath to introduce transitions between the states:

$$H_I = \sigma^x \otimes B \qquad B \text{ as usual,} \qquad \sigma^x = \sigma^+ + \sigma^- \tag{0.280}$$

Following the derivation in [2] we arrive at the equation

$$\begin{aligned}\dot{\boldsymbol{\rho}}_S(t) =& -i\left[\boldsymbol{H}_S^1(t), \mathrm{tr}_B\boldsymbol{\rho}(t)\right] - i\mathrm{tr}_B\left\{\left[\boldsymbol{H}_I(t), \boldsymbol{\rho}(0)\right]\right\} \\ & - \int_0^t \mathrm{tr}_B\left\{\left[\boldsymbol{H}_I(t)\left[\boldsymbol{H}_I(t'), \boldsymbol{\rho}(t')\right]\right]\right\} dt' - \int_0^t \mathrm{tr}_B\left\{\left[\boldsymbol{H}_I(t)\left[\boldsymbol{H}_S^1(t'), \boldsymbol{\rho}(t')\right]\right]\right\} dt'\end{aligned}$$

The second terms in each line vanish since they are linear in the bath operators and the trace thus yields zero, leaving us with the first and third term. We already know the third term from our usual considerations and know that it yields the Redfield-II equation with

$$\boldsymbol{A}_I(t) = e^{i(H_S^0 + H_B)t}\sigma^x e^{-i(H_S^0 + H_B)t} = \sigma^x \tag{0.281}$$

So that we are left with

$$\dot{\boldsymbol{\rho}}_S(t) = -i\left[\boldsymbol{H}_S^1(t), \boldsymbol{\rho}_S(t)\right] - \int_0^\infty \left\{\left[\sigma^x, \sigma^x \boldsymbol{\rho}_{\boldsymbol{S}}(t)\right] C(\tau) + h.c.\right\} d\tau \tag{0.282}$$

Performing the τ-Integration yields a very simple Lindblad-Equation

$$\dot{\boldsymbol{\rho}}_S(t) = -i\left[\boldsymbol{H}_S^1(t), \boldsymbol{\rho}_S(t)\right] + \gamma(0)\left\{\sigma^x \boldsymbol{\rho}_S(t)\sigma^x - \boldsymbol{\rho}_S(t)\right\} \tag{0.283}$$

Which is in Schrödinger picture just

$$\dot{\rho}_S(t) = -i\left[H_S(t), \rho_S(t)\right] + \gamma(0)\left\{\sigma^x \rho_S(t)\sigma^x - \rho_S(t)\right\} \tag{0.284}$$

The dynamics of $\langle P_{0/1}\rangle$ are at least not trivial:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{dt}}\langle P_0\rangle &= \mathrm{tr}\left\{P_0\dot{\rho}_S\right\} = \gamma(0)\mathrm{tr}\left\{P_0\sigma^x\rho_S\sigma^x - P_1\rho_S\right\} \\ &= \gamma(0)\mathrm{tr}\left\{\sigma^x\sigma^-\rho_S - P_0\rho_S\right\} = \gamma(0)\mathrm{tr}\left\{P_1\rho_S - P_0\rho_S\right\} \\ &= \gamma(0)\mathrm{tr}\left\{(1 - 2P_0)\rho_S\right\} \\ &= \gamma(0)(1 - 2\langle P_0\rangle)\end{aligned}$$

Which has the solution

$$\langle P_0 \rangle = P_0^0 e^{-2\gamma(0)t} + \frac{1}{2} \tag{0.285}$$

So the probability to be in one state relaxes to 1/2 with time. Interesting is also that the dynamics of $\langle \sigma^x \rangle$ seem to be dependent on $\langle x \rangle$:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{dt}}\langle \sigma^x \rangle &= -i\mathrm{tr}\left\{\sigma^x \left[\lambda \sigma^z \otimes (a + a^\dagger), \rho_S\right]\right\} \\
&\quad + \gamma(0)\mathrm{tr}\left\{\sigma^x \sigma^x \rho_S \sigma^x - \sigma^x \rho_S\right\} \\
&= -i\mathrm{tr}\left\{\lambda \sigma^x \sigma^z \otimes (a^\dagger + a)\rho_S - \lambda \sigma^x \rho_S \sigma^z \otimes (a^\dagger + a)\right\} \\
&= -i\mathrm{tr}\left\{\lambda \left(\sigma^x \sigma^z - \sigma^z \sigma^x\right) \otimes (a^\dagger + a)\rho_S\right\} = -2i\lambda \mathrm{tr}\left\{\left(\sigma^+ - \sigma^-\right) \otimes (a^\dagger + a)\rho_S\right\} \\
&= -2i\lambda \left(\langle \sigma^+ \rangle - \langle \sigma^- \rangle\right) \langle x \rangle \qquad \text{if} \quad \mathrm{tr}_{A+B}\left\{O_A \otimes O_B \rho_A \otimes \rho_B\right\} = \mathrm{tr}_A\left\{O_A \rho_A\right\} \mathrm{tr}_B\left\{O_B \rho_B\right\}
\end{aligned}$$

But I find that counter-intuitive that this depend on x and P_1 not.
Would it be reasonable to consider such a system for multiple lattice sites and introduce an "Ising-like" interaction

$$H_S^{\mu\nu} = J\sigma_\mu^z \sigma_\nu^z \tag{0.286}$$

and hope for interesting dynamics (that might even resemble my system?).
Interesting review article (kind of) about the dynamics of the dissipative two-state system, or spin-boson model: [1]. It even considers the possibility to approximate a double well system with a two state system. But it rather deals with short times and an approximation for oscillator energies much smaller than the double well.

0.3 Benchmarking

We need to make sure that our simulation leads to correct results, so we benchmark our system compared to analytically solvable cases. An important basic equation for this would be the Fokker-Planck-Equation:

$$\frac{\partial}{\partial t} p(x,t) = -\frac{\partial}{\partial x}(a(x,t)p(x,t)) + \frac{\partial^2}{\partial x^2}(D(x,t)p(x,t)) \tag{0.287}$$

Fokker-Planck-Equation is obtained from the master equation through something called the "Kramers-Moyal expansion". (Source: Wikipedia) Which describes the evolution of the probability density for a random Variable X_t to assume the value x at the time t. $a(x,t)$ is called the drift coefficient and $D(x,t)$ the diffusion coefficient. There is also a Version of the Fokker-Planck equation in higher dimensions, meaning if the random Variable $\mathbf{X_t}$ is a vector.