A general non-Markovian master equation for time-dependent Hamiltonians with coupling that is weak, strong, or anything in between

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I. THE HAMILTONIAN

We start with a time-dependent Hamiltonian of the form:

$$H(t) = H_S(t) + H_I + H_B, \tag{1}$$
$$H_S(t) = \varepsilon_0(t) |0\rangle\langle 0| + \varepsilon_1(t) |1\rangle\langle 1| + V_{10}(t) |1\rangle\langle 0| + V_{01}(t) |0\rangle\langle 1|, \tag{2}$$
$$H_I = |0\rangle\langle 0| \sum_{\mathbf{k}} \left(g_{0\mathbf{k}} b_{\mathbf{k}}^\dagger + g_{0\mathbf{k}}^* b_{\mathbf{k}} \right) + |1\rangle\langle 1| \sum_{\mathbf{k}} \left(g_{1\mathbf{k}} b_{\mathbf{k}}^\dagger + g_{1\mathbf{k}}^* b_{\mathbf{k}} \right), \tag{3}$$
$$H_B = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}. \tag{4}$$

For the states $|0\rangle, |1\rangle$ we have the ortonormal condition:

$$\langle i|j \rangle = \delta_{ij} \tag{5}$$

II. UNITARY TRANSFORMATION INTO THE VARIATIONALLY OPTIMIZABLE FRAME

We will apply to $H(t)$, the unitary transformation defined by $e^{\pm V}$ where is the variationally optimizable anti-Hermitian operator:

$$V \equiv |0\rangle\langle 0| \sum_{\mathbf{k}} \left(\alpha_{0\mathbf{k}} b_{\mathbf{k}}^\dagger - \alpha_{0\mathbf{k}}^* b_{\mathbf{k}} \right) + |1\rangle\langle 1| \sum_{\mathbf{k}} \left(\alpha_{1\mathbf{k}} b_{\mathbf{k}}^\dagger - \alpha_{1\mathbf{k}}^* b_{\mathbf{k}} \right) \tag{6}$$

in terms of the variational scalar parameters $v_{\mathbf{k}}$ defined as:

$$v_{n,\mathbf{k}} = \omega_{\mathbf{k}} \alpha_{n,\mathbf{k}} \tag{7}$$

which will soon be optimized in order to give the most accurate possible master equation for the system's dynamics in the presence of this bath. We define the following notation for the function (6):

$$\hat{\varphi}_n \equiv \sum_{\mathbf{k}} \left(\alpha_{n\mathbf{k}} b_{\mathbf{k}}^\dagger - \alpha_{n\mathbf{k}}^* b_{\mathbf{k}} \right), \tag{8}$$
$$V = |0\rangle\langle 0| \hat{\varphi}_0 + |1\rangle\langle 1| \hat{\varphi}_1. \tag{9}$$

Here $*$ denotes the complex conjugate. Expanding $e^{\pm V}$ using the notation (6)will give us the following result:

$$e^{\pm V} = e^{\pm(|0\rangle\langle 0|\hat{\varphi}_0 + |1\rangle\langle 1|\hat{\varphi}_1)} \tag{10}$$

$$= \mathbb{I} \pm (|0\rangle\langle 0|\hat{\varphi}_0 + |1\rangle\langle 1|\hat{\varphi}_1) + \frac{(\pm(|0\rangle\langle 0|\hat{\varphi}_0 + |1\rangle\langle 1|\hat{\varphi}_1))^2}{2!} + \ldots \tag{11}$$

$$= |0\rangle\langle 0| + |1\rangle\langle 1| \pm (|0\rangle\langle 0|\hat{\varphi}_0 + |1\rangle\langle 1|\hat{\varphi}_1) + \frac{|0\rangle\langle 0|\hat{\varphi}_0{}^2}{2!} + \frac{|1\rangle\langle 1|\hat{\varphi}_1{}^2}{2!} + \ldots \tag{12}$$

$$= |0\rangle\langle 0|\left(1 \pm \hat{\varphi}_0 + \frac{\hat{\varphi}_0{}^2}{2!} \pm \ldots\right) + |1\rangle\langle 1|\left(1 \pm \hat{\varphi}_1 + \frac{\hat{\varphi}_1{}^2}{2!} \pm \ldots\right) \tag{13}$$

$$= |0\rangle\langle 0|e^{\pm\hat{\varphi}_0} + |1\rangle\langle 1|e^{\pm\hat{\varphi}_1} \tag{14}$$

$$= |0\rangle\langle 0|e^{\pm\sum_{\mathbf{k}}\left(\alpha_{0\mathbf{k}}b_{\mathbf{k}}^\dagger - \alpha_{0\mathbf{k}}^* b_{\mathbf{k}}\right)} + |1\rangle\langle 1|e^{\pm\sum_{\mathbf{k}}\left(\alpha_{1\mathbf{k}}b_{\mathbf{k}}^\dagger - \alpha_{1\mathbf{k}}^* b_{\mathbf{k}}\right)} \tag{15}$$

$$= |0\rangle\langle 0|B_{0\pm} + |1\rangle\langle 1|B_{1\pm}, \tag{16}$$

$$B_{i\pm} \equiv e^{\pm\sum_{\mathbf{k}}\left(\alpha_{i\mathbf{k}}b_{\mathbf{k}}^\dagger - \alpha_{i\mathbf{k}}^* b_{\mathbf{k}}\right)}. \tag{17}$$

Let's recall the Zassenhaus formula:

$$e^{t(X+Y)} = e^{tX}\, e^{tY}\, e^{-\frac{t^2}{2}[X,Y]}\, e^{\frac{t^3}{6}(2[Y,[X,Y]]+[X,[X,Y]])}\, e^{\frac{-t^4}{24}([[[X,Y],X],X]+3[[[X,Y],X],Y]+3[[[X,Y],Y],Y])} \cdots \tag{18}$$

Since $\left[\alpha_{i\mathbf{k}}b_{\mathbf{k}}^\dagger - \alpha_{i\mathbf{k}}^* b_{\mathbf{k}}, \alpha_{j\mathbf{k}'}b_{\mathbf{k}'}^\dagger - \alpha_{j\mathbf{k}'}^* b_{\mathbf{k}'}\right] = 0$ for all $\mathbf{k}', \mathbf{k}$, we can show making $t = 1$ in (18) the following result:

$$e^{\left(\alpha_{i\mathbf{k}}b_{\mathbf{k}}^\dagger - \alpha_{i\mathbf{k}}^* b_{\mathbf{k}}\right) + \left(\alpha_{j\mathbf{k}'}b_{\mathbf{k}'}^\dagger - \alpha_{j\mathbf{k}'}^* b_{\mathbf{k}'}\right)} = e^{\alpha_{i\mathbf{k}}b_{\mathbf{k}}^\dagger - \alpha_{i\mathbf{k}}^* b_{\mathbf{k}}} e^{\alpha_{j\mathbf{k}'}b_{\mathbf{k}'}^\dagger - \alpha_{j\mathbf{k}'}^* b_{\mathbf{k}'}} e^{-\frac{1}{2}\left[\alpha_{i\mathbf{k}}b_{\mathbf{k}}^\dagger - \alpha_{i\mathbf{k}}^* b_{\mathbf{k}}, \alpha_{j\mathbf{k}'}b_{\mathbf{k}'}^\dagger - \alpha_{j\mathbf{k}'}^* b_{\mathbf{k}'}\right]} \cdots \tag{19}$$

$$= e^{\alpha_{i\mathbf{k}}b_{\mathbf{k}}^\dagger - \alpha_{i\mathbf{k}}^* b_{\mathbf{k}}} e^{\alpha_{j\mathbf{k}'}b_{\mathbf{k}'}^\dagger - \alpha_{j\mathbf{k}'}^* b_{\mathbf{k}'}} e^{-\frac{1}{2} 0} \cdots \tag{20}$$

$$= e^{\alpha_{i\mathbf{k}}b_{\mathbf{k}}^\dagger - \alpha_{i\mathbf{k}}^* b_{\mathbf{k}}} e^{\alpha_{j\mathbf{k}'}b_{\mathbf{k}'}^\dagger - \alpha_{j\mathbf{k}'}^* b_{\mathbf{k}'}} \tag{21}$$

By induction of this result we can write expresion of $B_{i\pm}$ as a product of exponentials, which we will call "displacement" operators $D\left(\pm\alpha_{i\mathbf{k}}\right)$:

$$B_{i\pm} = \prod_{\mathbf{k}} D\left(\pm\alpha_{i\mathbf{k}}\right), \tag{22}$$

$$D\left(\pm\alpha_{i\mathbf{k}}\right) \equiv e^{\pm\left(\alpha_{i\mathbf{k}}b_{\mathbf{k}}^\dagger - \alpha_{i\mathbf{k}}^* b_{\mathbf{k}}\right)}. \tag{23}$$

this will help us to write operators O in the variational frame :

$$\overline{O} \equiv e^V O e^{-V}. \tag{24}$$

We use the following identities:

$$\overline{|0\rangle\langle0|} = \mathrm{e}^{V}|0\rangle\langle0|\mathrm{e}^{-V} \tag{25}$$

$$= \left(|0\rangle\langle0|B_{0+} + |1\rangle\langle1|B_{1+}\right)|0\rangle\langle0|\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{26}$$

$$= \left(|0\rangle\langle0|0\rangle\langle0|B_{0+} + |1\rangle\langle1|0\rangle\langle0|B_{1+}\right)\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{27}$$

$$= |0\rangle\langle0|0\rangle\langle0|B_{0+}\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{28}$$

$$= |0\rangle\langle0|B_{0+}\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{29}$$

$$= |0\rangle\langle0|0\rangle\langle0|B_{0+}B_{0-} + |0\rangle\langle0|1\rangle\langle1|B_{0+}B_{1-} \tag{30}$$

$$= |0\rangle\langle0| \tag{31}$$

$$\overline{|1\rangle\langle1|} = \left(|0\rangle\langle0|B_{0+} + |1\rangle\langle1|B_{1+}\right)|1\rangle\langle1|\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{32}$$

$$= \left(|0\rangle\langle0|1\rangle\langle1|B_{0+} + |1\rangle\langle1|1\rangle\langle1|B_{1+}\right)\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{33}$$

$$= |1\rangle\langle1|B_{1+}\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{34}$$

$$= |1\rangle\langle1|0\rangle\langle0|B_{1+}B_{0-} + B_{1+}|1\rangle\langle1|1\rangle\langle1|B_{1-} \tag{35}$$

$$= B_{1+}|1\rangle\langle1|1\rangle\langle1|B_{1-} \tag{36}$$

$$= |1\rangle\langle1|B_{1+}B_{1-} \tag{37}$$

$$= |1\rangle\langle1| \tag{38}$$

$$\overline{|0\rangle\langle1|} = \mathrm{e}^{V}|0\rangle\langle1|\mathrm{e}^{-V} \tag{39}$$

$$= \left(|0\rangle\langle0|B_{0+} + |1\rangle\langle1|B_{1+}\right)|0\rangle\langle1|\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{40}$$

$$= \left(|0\rangle\langle0|0\rangle\langle1|B_{0+} + |1\rangle\langle1|B_{1+}|0\rangle\langle1|\right)\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{41}$$

$$= \left(|0\rangle\langle0|0\rangle\langle1|B_{0+} + |1\rangle\langle1|0\rangle\langle1|B_{1+}\right)\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{42}$$

$$= |0\rangle\langle1|B_{0+}\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{43}$$

$$= |0\rangle\langle1|0\rangle\langle0|B_{0+}B_{0-} + |0\rangle\langle1|1\rangle\langle1|B_{0+}B_{1-} \tag{44}$$

$$= |0\rangle\langle1|B_{0+}B_{1-} \tag{45}$$

$$\overline{|1\rangle\langle0|} = \mathrm{e}^{V}|1\rangle\langle0|\mathrm{e}^{-V} \tag{46}$$

$$= \left(|0\rangle\langle0|B_{0+} + |1\rangle\langle1|B_{1+}\right)|1\rangle\langle0|\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{47}$$

$$= \left(|0\rangle\langle0|1\rangle\langle0|B_{0+} + |1\rangle\langle1|B_{1+}|1\rangle\langle0|\right)\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{48}$$

$$= \left(|0\rangle\langle0|1\rangle\langle0|B_{0+} + |1\rangle\langle1|1\rangle\langle0|B_{1+}\right)\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{49}$$

$$= |1\rangle\langle0|B_{1+}\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{50}$$

$$= |1\rangle\langle0|B_{1+}|0\rangle\langle0|B_{0-} + |1\rangle\langle0|B_{1+}|1\rangle\langle1|B_{1-} \tag{51}$$

$$= |1\rangle\langle0|B_{1+}B_{0-} + |1\rangle\langle0|1\rangle\langle1|B_{1+}B_{1-} \tag{52}$$

$$= |1\rangle\langle0|B_{1+}B_{0-} \tag{53}$$

$$\overline{b_{\mathbf{k}}} = \mathrm{e}^{V}b_{\mathbf{k}}\mathrm{e}^{-V} \tag{54}$$

$$= \left(|0\rangle\langle0|B_{0+} + |1\rangle\langle1|B_{1+}\right)b_{\mathbf{k}}\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{55}$$

$$= |0\rangle\langle0|B_{0+}b_{\mathbf{k}}B_{0-}|0\rangle\langle0| + |0\rangle\langle0|B_{0+}b_{\mathbf{k}}|1\rangle\langle1|B_{1-} + |1\rangle\langle1|B_{1+}b_{\mathbf{k}}|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1+}b_{\mathbf{k}}B_{1-}|1\rangle\langle1| \tag{56}$$

$$= |0\rangle\langle0|0\rangle\langle0|B_{0+}b_{\mathbf{k}}B_{0-} + |0\rangle\langle0|1\rangle\langle1|B_{0+}b_{\mathbf{k}}B_{1-} + |1\rangle\langle1|0\rangle\langle0|B_{1+}b_{\mathbf{k}}B_{0-} + |1\rangle\langle1|B_{1+}b_{\mathbf{k}}B_{1-} \tag{57}$$

$$= |0\rangle\langle0|\left(b_{\mathbf{k}} - \alpha_{0\mathbf{k}}\right) + |1\rangle\langle1|\left(b_{\mathbf{k}} - \alpha_{1\mathbf{k}}\right) \tag{58}$$

$$= \left(|0\rangle\langle0| + |1\rangle\langle1|\right)b_{\mathbf{k}} - |1\rangle\langle1|\alpha_{1\mathbf{k}} - |0\rangle\langle0|\alpha_{0\mathbf{k}} \tag{59}$$

$$= b_{\mathbf{k}} - |1\rangle\langle1|\alpha_{1\mathbf{k}} - |0\rangle\langle0|\alpha_{0\mathbf{k}} \tag{60}$$

$$\overline{b_{\mathbf{k}}}^{\dagger} = \mathrm{e}^{V}b_{\mathbf{k}}^{\dagger}\mathrm{e}^{-V} \tag{61}$$

$$= \left(|0\rangle\langle0|B_{0+} + |1\rangle\langle1|B_{1+}\right)b_{\mathbf{k}}^{\dagger}\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{62}$$

$$= |0\rangle\langle0|B_{0+}b_{\mathbf{k}}^{\dagger}B_{0-}|0\rangle\langle0| + |0\rangle\langle0|B_{0+}b_{\mathbf{k}}^{\dagger}|1\rangle\langle1|B_{1-} + |1\rangle\langle1|B_{1+}b_{\mathbf{k}}^{\dagger}|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1+}b_{\mathbf{k}}^{\dagger}B_{1-}|1\rangle\langle1| \tag{63}$$

$$= |0\rangle\langle0|0\rangle\langle0|B_{0+}b_{\mathbf{k}}^{\dagger}B_{0-} + |0\rangle\langle0|1\rangle\langle1|B_{0+}b_{\mathbf{k}}^{\dagger}B_{1-} + |1\rangle\langle1|0\rangle\langle0|B_{1+}b_{\mathbf{k}}^{\dagger}B_{0-} + |1\rangle\langle1|B_{1+}b_{\mathbf{k}}^{\dagger}B_{1-} \tag{64}$$

$$= |0\rangle\langle0|\left(b_{\mathbf{k}}^{\dagger} - \alpha_{0\mathbf{k}}^{*}\right) + |1\rangle\langle1|\left(b_{\mathbf{k}}^{\dagger} - \alpha_{1\mathbf{k}}^{*}\right) \tag{65}$$

$$= \left(|0\rangle\langle0| + |1\rangle\langle1|\right)b_{\mathbf{k}}^{\dagger} - |1\rangle\langle1|\alpha_{1\mathbf{k}}^{*} - |0\rangle\langle0|\alpha_{0\mathbf{k}}^{*} \tag{66}$$

$$= b_{\mathbf{k}} - |1\rangle\langle1|\alpha_{1\mathbf{k}}^{*} - |0\rangle\langle0|\alpha_{0\mathbf{k}}^{*} \tag{67}$$

We have used the following:

$$B_{i+} b_{\mathbf{k}} B_{i-} = b_{\mathbf{k}} - \alpha_{i\mathbf{k}} \tag{68}$$

$$B_{i+} b_{\mathbf{k}}^{\dagger} B_{i-} = b_{\mathbf{k}}^{\dagger} - \alpha_{i\mathbf{k}}^{*} \tag{69}$$

We therefore have the following relationships:

$$\overline{\varepsilon_0\left(t\right)|0\rangle\langle0|} = \varepsilon_0\left(t\right)|0\rangle\langle0| \tag{70}$$

$$\overline{\varepsilon_1\left(t\right)|1\rangle\langle1|} = \varepsilon_1\left(t\right)|1\rangle\langle1| \tag{71}$$

$$\overline{V_{10}\left(t\right)|1\rangle\langle0|} = V_{10}\left(t\right)|1\rangle\langle0|B_{1+}B_{0-} \tag{72}$$

$$\overline{V_{01}\left(t\right)|0\rangle\langle1|} = V_{01}\left(t\right)|0\rangle\langle1|B_{0+}B_{1-} \tag{73}$$

$$\overline{g_{i\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{i\mathbf{k}}^* b_{\mathbf{k}}} = g_{i\mathbf{k}}\left(|0\rangle\langle0|\left(b_{\mathbf{k}}^\dagger - \alpha_{0\mathbf{k}}^*\right) + |1\rangle\langle1|\left(b_{\mathbf{k}}^\dagger - \alpha_{1\mathbf{k}}^*\right)\right) + g_{i\mathbf{k}}^*\left(|0\rangle\langle0|\left(b_{\mathbf{k}} - \alpha_{0\mathbf{k}}\right) + |1\rangle\langle1|\left(b_{\mathbf{k}} - \alpha_{1\mathbf{k}}\right)\right) \tag{74}$$

$$= g_{i\mathbf{k}}\left(\left(|0\rangle\langle0| + |1\rangle\langle1|\right)b_{\mathbf{k}}^\dagger - \alpha_{1\mathbf{k}}^*|1\rangle\langle1| - \alpha_{0\mathbf{k}}^*|0\rangle\langle0|\right) \tag{75}$$

$$+ g_{i\mathbf{k}}^*\left(\left(|0\rangle\langle0| + |1\rangle\langle1|\right)b_{\mathbf{k}}^\dagger - \alpha_{1\mathbf{k}}|1\rangle\langle1| - \alpha_{0\mathbf{k}}|0\rangle\langle0|\right) \tag{76}$$

$$= g_{i\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{i\mathbf{k}}^* b_{\mathbf{k}} - g_{i\mathbf{k}}\alpha_{0\mathbf{k}}^*|0\rangle\langle0| - g_{i\mathbf{k}}^*\alpha_{0\mathbf{k}}|0\rangle\langle0| - g_{i\mathbf{k}}\alpha_{1\mathbf{k}}^*|1\rangle\langle1| - g_{i\mathbf{k}}^*\alpha_{1\mathbf{k}}|1\rangle\langle1| \tag{77}$$

$$= g_{i\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{i\mathbf{k}}^* b_{\mathbf{k}} - \left(g_{i\mathbf{k}}\alpha_{0\mathbf{k}}^* + g_{i\mathbf{k}}^*\alpha_{0\mathbf{k}}\right)|0\rangle\langle0| - \left(g_{i\mathbf{k}}\alpha_{1\mathbf{k}}^* + g_{i\mathbf{k}}^*\alpha_{1\mathbf{k}}\right)|1\rangle\langle1| \tag{78}$$

$$\overline{|0\rangle\langle0|\left(g_{0\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{0\mathbf{k}}^* b_{\mathbf{k}}\right)} = \left(|0\rangle\langle0|B_{0+} + |1\rangle\langle1|B_{1+}\right)|0\rangle\langle0|\left(g_{0\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{0\mathbf{k}}^* b_{\mathbf{k}}\right)\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{79}$$

$$= |0\rangle\langle0|B_{0+}|0\rangle\langle0|\left(g_{0\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{0\mathbf{k}}^* b_{\mathbf{k}}\right)|0\rangle\langle0|B_{0-} \tag{80}$$

$$= |0\rangle\langle0|B_{0+}\left(g_{0\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{0\mathbf{k}}^* b_{\mathbf{k}}\right)B_{0-} \tag{81}$$

$$= |0\rangle\langle0|\left(g_{0\mathbf{k}}\left(b_{\mathbf{k}}^\dagger - \alpha_{0\mathbf{k}}^*\right) + g_{0\mathbf{k}}^*\left(b_{\mathbf{k}} - \alpha_{0\mathbf{k}}\right)\right) \tag{82}$$

$$\overline{|1\rangle\langle1|\left(g_{1\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{1k}^* b_{\mathbf{k}}\right)} = \left(|0\rangle\langle0|B_{0+} + |1\rangle\langle1|B_{1+}\right)|1\rangle\langle1|\left(g_{1\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{1k}^* b_{\mathbf{k}}\right)\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{83}$$

$$= |1\rangle\langle1|B_{1+}|1\rangle\langle1|\left(g_{1\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{1k}^* b_{\mathbf{k}}\right)|1\rangle\langle1|B_{1-} \tag{84}$$

$$= |1\rangle\langle1|B_{1+}\left(g_{1\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{1\mathbf{k}}^* b_{\mathbf{k}}\right)B_{1-} \tag{85}$$

$$= |1\rangle\langle1|\left(g_{1\mathbf{k}}\left(b_{\mathbf{k}}^\dagger - \alpha_{1\mathbf{k}}^*\right) + g_{1\mathbf{k}}^*\left(b_{\mathbf{k}} - \alpha_{1\mathbf{k}}\right)\right) \tag{86}$$

$$\overline{\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}}} = \omega_{\mathbf{k}}\left(|0\rangle\langle0|B_{0+} + |1\rangle\langle1|B_{1+}\right)b_{\mathbf{k}}^\dagger b_{\mathbf{k}}\left(|0\rangle\langle0|B_{0-} + |1\rangle\langle1|B_{1-}\right) \tag{87}$$

$$= \omega_{\mathbf{k}}\left(|0\rangle\langle0|\prod_{\mathbf{k}'}D\left(\alpha_{0\mathbf{k}'}\right) + |1\rangle\langle1|\prod_{\mathbf{k}'}D\left(\alpha_{1\mathbf{k}'}\right)\right)b_{\mathbf{k}}^\dagger b_{\mathbf{k}}\left(|0\rangle\langle0|\prod_{\mathbf{k}'}D\left(-\alpha_{0\mathbf{k}'}\right) + |1\rangle\langle1|\prod_{\mathbf{k}'}D\left(-\alpha_{1\mathbf{k}'}\right)\right) \tag{88}$$

$$= \omega_{\mathbf{k}}\left(|0\rangle\langle0|\prod_{\mathbf{k}'}D\left(\alpha_{0\mathbf{k}'}\right)b_{\mathbf{k}}^\dagger b_{\mathbf{k}}\prod_{\mathbf{k}'}D\left(-\alpha_{0\mathbf{k}'}\right)|0\rangle\langle0| + |0\rangle\langle0|\prod_{\mathbf{k}'}D\left(\alpha_{0\mathbf{k}'}\right)b_{\mathbf{k}}^\dagger b_{\mathbf{k}}|1\rangle\langle1|\prod_{\mathbf{k}'}D\left(-\alpha_{1\mathbf{k}'}\right)\right. \tag{89}$$

$$\left. + |1\rangle\langle1|D\left(\alpha_{1\mathbf{k}}\right)b_{\mathbf{k}}^\dagger b_{\mathbf{k}}D\left(-\alpha_{1\mathbf{k}}\right)\prod_{\mathbf{k}'\neq\mathbf{k}}D\left(\alpha_{1\mathbf{k}'}\right)\prod_{\mathbf{k}'\neq\mathbf{k}}D\left(-\alpha_{1\mathbf{k}'}\right)\right) \tag{90}$$

$$= \omega_{\mathbf{k}}\left(|0\rangle\langle0|D\left(\alpha_{0\mathbf{k}}\right)b_{\mathbf{k}}^\dagger b_{\mathbf{k}}D\left(-\alpha_{0\mathbf{k}}\right)\prod_{\mathbf{k}'\neq\mathbf{k}}D\left(\alpha_{0\mathbf{k}'}\right)\prod_{\mathbf{k}'\neq\mathbf{k}}D\left(-\alpha_{0\mathbf{k}'}\right)\right. \tag{91}$$

$$\left. + |1\rangle\langle1|D\left(\alpha_{1\mathbf{k}}\right)b_{\mathbf{k}}^\dagger b_{\mathbf{k}}D\left(-\alpha_{1\mathbf{k}}\right)\prod_{\mathbf{k}'\neq\mathbf{k}}D\left(\alpha_{1\mathbf{k}'}\right)\prod_{\mathbf{k}'\neq\mathbf{k}}D\left(-\alpha_{1\mathbf{k}'}\right)\right) \tag{92}$$

$$= \omega_{\mathbf{k}}\left(|0\rangle\langle0|D\left(\alpha_{0\mathbf{k}}\right)b_{\mathbf{k}}^\dagger b_{\mathbf{k}}D\left(-\alpha_{0\mathbf{k}}\right)\mathbb{I} + |1\rangle\langle1|D\left(\alpha_{1\mathbf{k}}\right)b_{\mathbf{k}}^\dagger b_{\mathbf{k}}D\left(-\alpha_{1\mathbf{k}}\right)\mathbb{I}\right) \tag{93}$$

$$= \omega_{\mathbf{k}}\left(|0\rangle\langle0|\left(b_{\mathbf{k}}^\dagger - \alpha_{0\mathbf{k}}^*\right)\left(b_{\mathbf{k}} - \alpha_{0\mathbf{k}}\right) + |1\rangle\langle1|\left(b_{\mathbf{k}}^\dagger - \alpha_{1\mathbf{k}}^*\right)\left(b_{\mathbf{k}} - \alpha_{1\mathbf{k}}\right)\right) \tag{94}$$

$$= \omega_{\mathbf{k}}\left(|0\rangle\langle0|\left(b_{\mathbf{k}}^\dagger b_{\mathbf{k}} - \alpha_{0\mathbf{k}}^* b_{\mathbf{k}} - \alpha_{0\mathbf{k}}b_{\mathbf{k}}^\dagger + |\alpha_{0\mathbf{k}}|^2\right) + |1\rangle\langle1|\left(b_{\mathbf{k}}^\dagger b_{\mathbf{k}} - \alpha_{1\mathbf{k}}^* b_{\mathbf{k}} - \alpha_{1\mathbf{k}}b_{\mathbf{k}}^\dagger + |\alpha_{1\mathbf{k}}|^2\right)\right) \tag{95}$$

$$= \omega_{\mathbf{k}}\left(|0\rangle\langle0|\left(b_{\mathbf{k}}^\dagger b_{\mathbf{k}} - \alpha_{0\mathbf{k}}^* b_{\mathbf{k}} - \alpha_{0\mathbf{k}}b_{\mathbf{k}}^\dagger + |\alpha_{0\mathbf{k}}|^2\right) + |1\rangle\langle1|\left(b_{\mathbf{k}}^\dagger b_{\mathbf{k}} - \alpha_{1\mathbf{k}}^* b_{\mathbf{k}} - \alpha_{1\mathbf{k}}b_{\mathbf{k}}^\dagger + |\alpha_{1\mathbf{k}}|^2\right)\right) \tag{96}$$

$$= \omega_{\mathbf{k}}\left(|0\rangle\langle0|b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + |1\rangle\langle1|b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + |1\rangle\langle1|\left(|\alpha_{1\mathbf{k}}|^2 - b_{\mathbf{k}}^\dagger\alpha_{1\mathbf{k}} - b_{\mathbf{k}}\alpha_{1\mathbf{k}}^*\right)\right) \tag{97}$$

$$+ \omega_{\mathbf{k}}|0\rangle\langle0|\left(|\alpha_{0\mathbf{k}}|^2 - b_{\mathbf{k}}^\dagger\alpha_{0\mathbf{k}} - b_{\mathbf{k}}\alpha_{0\mathbf{k}}^*\right) \tag{98}$$

$$= \omega_{\mathbf{k}} \left((|0\rangle\langle 0| + |1\rangle\langle 1|) \, b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + |1\rangle\langle 1| \left(|\alpha_{1\mathbf{k}}|^2 - b_{\mathbf{k}}^{\dagger} \alpha_{1\mathbf{k}} - b_{\mathbf{k}} \alpha_{1\mathbf{k}}^* \right) \right) \tag{99}$$

$$+ \omega_{\mathbf{k}} |0\rangle\langle 0| \left(|\alpha_{0\mathbf{k}}|^2 - b_{\mathbf{k}}^{\dagger} \alpha_{0\mathbf{k}} - b_{\mathbf{k}} \alpha_{0\mathbf{k}}^* \right) \tag{100}$$

$$= \omega_{\mathbf{k}} \left((|0\rangle\langle 0| + |1\rangle\langle 1|) \, b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + |1\rangle\langle 1| \left(|\alpha_{1\mathbf{k}}|^2 - \left(b_{\mathbf{k}}^{\dagger} \alpha_{1\mathbf{k}} + b_{\mathbf{k}} \alpha_{1\mathbf{k}}^* \right) \right) \right) \tag{101}$$

$$+ \omega_{\mathbf{k}} |0\rangle\langle 0| \left(|\alpha_{0\mathbf{k}}|^2 - \left(b_{\mathbf{k}}^{\dagger} \alpha_{0\mathbf{k}} + b_{\mathbf{k}} \alpha_{0\mathbf{k}}^* \right) \right) \tag{102}$$

$$= \omega_{\mathbf{k}} \left(|b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + |1\rangle\langle 1| \left(|\alpha_{1\mathbf{k}}|^2 - \left(b_{\mathbf{k}}^{\dagger} \alpha_{1\mathbf{k}} + b_{\mathbf{k}} \alpha_{1\mathbf{k}}^* \right) \right) + |0\rangle\langle 0| \left(|\alpha_{0\mathbf{k}}|^2 - \left(b_{\mathbf{k}}^{\dagger} \alpha_{0\mathbf{k}} + b_{\mathbf{k}} \alpha_{0\mathbf{k}}^* \right) \right) \right) \tag{103}$$

So all parts of $H(t)$ can be written in the variationally optimizable frame now:

$$\overline{H_S(t)} = \overline{\varepsilon_0 (t) |0\rangle\langle 0|} + \overline{\varepsilon_1 (t) |1\rangle\langle 1|} + \overline{V_{10} (t) |1\rangle\langle 0|} + \overline{V_{01} (t) |0\rangle\langle 1|} \tag{104}$$

$$= \varepsilon_0 (t) |0\rangle\langle 0| + \varepsilon_1 (t) |1\rangle\langle 1| + V_{10} (t) |1\rangle\langle 0| B_{1+} B_{0-} + V_{01} (t) |0\rangle\langle 1| B_{0+} B_{1-} \tag{105}$$

$$\overline{H_I} = \overline{\sum_{\mathbf{k}} |0\rangle\langle 0| \left(g_{0\mathbf{k}} b_{\mathbf{k}}^{\dagger} + g_{0\mathbf{k}}^* b_{\mathbf{k}} \right)} + \overline{\sum_{\mathbf{k}} |1\rangle\langle 1| \left(g_{1\mathbf{k}} b_{\mathbf{k}}^{\dagger} + g_{1\mathbf{k}}^* b_{\mathbf{k}} \right)} \tag{106}$$

$$= \sum_{\mathbf{k}} |0\rangle\langle 0| \overline{\left(g_{0\mathbf{k}} b_{\mathbf{k}}^{\dagger} + g_{0\mathbf{k}}^* b_{\mathbf{k}} \right)} + \sum_{\mathbf{k}} |1\rangle\langle 1| \overline{\left(g_{1\mathbf{k}} b_{\mathbf{k}}^{\dagger} + g_{1\mathbf{k}}^* b_{\mathbf{k}} \right)} \tag{107}$$

$$= \sum_{\mathbf{k}} |0\rangle\langle 0| \left(g_{0\mathbf{k}} \left(b_{\mathbf{k}}^{\dagger} - \alpha_{0\mathbf{k}}^* \right) + g_{0\mathbf{k}}^* (b_{\mathbf{k}} - \alpha_{0\mathbf{k}}) \right) \tag{108}$$

$$+ \sum_{\mathbf{k}} |1\rangle\langle 1| \left(g_{1\mathbf{k}} \left(b_{\mathbf{k}}^{\dagger} - \alpha_{1\mathbf{k}}^* \right) + g_{1\mathbf{k}}^* (b_{\mathbf{k}} - \alpha_{1\mathbf{k}}) \right) \tag{109}$$

$$\overline{H_B} = \overline{\sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}} \tag{110}$$

$$= \sum_{\mathbf{k}} \overline{\omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}} \tag{111}$$

$$= \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(|b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + |1\rangle\langle 1| \left(|\alpha_{1\mathbf{k}}|^2 - \left(b_{\mathbf{k}}^{\dagger} \alpha_{1\mathbf{k}} + b_{\mathbf{k}} \alpha_{1\mathbf{k}}^* \right) \right) + |0\rangle\langle 0| \left(|\alpha_{0\mathbf{k}}|^2 - \left(b_{\mathbf{k}}^{\dagger} \alpha_{0\mathbf{k}} + b_{\mathbf{k}} \alpha_{0\mathbf{k}}^* \right) \right) \right) \tag{112}$$

Finally merging these expressions gives the transformed Hamiltonian:

$$\overline{H(t)} = \varepsilon_0 (t) |0\rangle\langle 0| + \varepsilon_1 (t) |1\rangle\langle 1| + V_{10} (t) |1\rangle\langle 0| B_{1+} B_{0-} + V_{01} (t) |0\rangle\langle 1| B_{0+} B_{1-} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} \tag{113}$$

$$+ \sum_{\mathbf{k}} \left(|0\rangle\langle 0| \left((g_{0\mathbf{k}} - \omega_{\mathbf{k}} \alpha_{0\mathbf{k}}) \, b_{\mathbf{k}}^{\dagger} + (g_{0\mathbf{k}} - \omega_{\mathbf{k}} \alpha_{0\mathbf{k}})^* b_{\mathbf{k}} \right) + |1\rangle\langle 1| \left((g_{1\mathbf{k}} - \omega_{\mathbf{k}} \alpha_{1\mathbf{k}}) \, b_{\mathbf{k}}^{\dagger} + (g_{1\mathbf{k}} - \omega_{\mathbf{k}} \alpha_{1\mathbf{k}})^* b_{\mathbf{k}} \right) \right) \tag{114}$$

$$+ \sum_{\mathbf{k}} \left(|0\rangle\langle 0| \left(\omega_{\mathbf{k}} |\alpha_{0\mathbf{k}}|^2 - (g_{0\mathbf{k}} \alpha_{0\mathbf{k}}^* + g_{0\mathbf{k}}^* \alpha_{0\mathbf{k}}) \right) + |1\rangle\langle 1| \left(\omega_{\mathbf{k}} |\alpha_{1\mathbf{k}}|^2 - (g_{1\mathbf{k}} \alpha_{1\mathbf{k}}^* + g_{1\mathbf{k}}^* \alpha_{1\mathbf{k}}) \right) \right) \tag{115}$$

Also we may write this transformed Hamiltonian as a sum of the form:

$$\overline{H(t)} = \overline{H_{\tilde{S}}} + \overline{H_{\tilde{I}}} + \overline{H_{\tilde{B}}} \tag{116}$$

Let's define:

$$R_i \equiv \sum_{\mathbf{k}} \left(\omega_{\mathbf{k}} |\alpha_{i\mathbf{k}}|^2 - (g_{i\mathbf{k}} \alpha_{i\mathbf{k}}^* + g_{i\mathbf{k}}^* \alpha_{i\mathbf{k}}) \right) \tag{117}$$

$$B_{iz} \equiv \sum_{\mathbf{k}} \left((g_{i\mathbf{k}} - v_{i\mathbf{k}}) \, b_{\mathbf{k}}^{\dagger} + (g_{i\mathbf{k}} - v_{i\mathbf{k}})^* b_{\mathbf{k}} \right) \tag{118}$$

We assume that the bath is at equilibrium with inverse temperature $\beta = 1/k_{\mathrm{B}}T$:

$$\rho_B = \frac{e^{-\beta H_B}}{\mathrm{Tr}\left(e^{-\beta H_B}\right)} \tag{119}$$

We can show using the coherence representation of the creation and annihilation operators that:

$$b_{\mathbf{k}}^{\dagger} = \begin{pmatrix} 0 & 0 & 0 & \ldots & 0 & \ldots \\ \sqrt{1} & 0 & 0 & \ldots & 0 & \ldots \\ 0 & \sqrt{2} & 0 & \ldots & 0 & \ldots \\ 0 & 0 & \sqrt{3} & \ldots & 0 & \ldots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ldots \\ 0 & 0 & 0 & \ldots & \sqrt{n} & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{120}$$

$$b_{\mathbf{k}} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \ldots & 0 & \ldots \\ 0 & 0 & \sqrt{2} & 0 & \ldots & 0 & \ldots \\ 0 & 0 & 0 & \sqrt{3} & \ldots & 0 & \ldots \\ 0 & 0 & 0 & 0 & \ddots & \vdots & \ldots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \sqrt{n} & \ldots \\ 0 & 0 & 0 & 0 & \ldots & 0 & \ddots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{121}$$

So the product of the matrix representation of $b_{\mathbf{k}}^{\dagger}$ and $b_{\mathbf{k}}$ is:

$$-\beta\omega_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}} = -\beta\omega_{\mathbf{k}} \begin{pmatrix} 0 & 0 & 0 & \ldots & 0 & \ldots \\ 0 & 1 & 0 & \ldots & 0 & \ldots \\ 0 & 0 & 2 & \ldots & 0 & \ldots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ldots \\ 0 & 0 & 0 & \ldots & n & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{122}$$

$$= \sum_{j=0}^{\infty} -j\beta\omega_{\mathbf{k}} \left|j\right\rangle \left\langle j\right| \tag{123}$$

So the density matrix ρ_B written in the coherence representation can be obtained using the Zassenhaus formula and the fact that $\left[\left|j\right\rangle \left\langle j\right|, \left|i\right\rangle \left\langle i\right|\right] = 0$ for all i, j.

$$\exp\left(-\beta\omega_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}\right) = \sum_{j_{\mathbf{k}}} \exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right) \left|j_{\mathbf{k}}\right\rangle \left\langle j_{\mathbf{k}}\right| \tag{124}$$

$$\exp\left(-\beta\sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}\right) = \prod_{k}\sum_{j_{\mathbf{k}}} \exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right) \left|j_{\mathbf{k}}\right\rangle \left\langle j_{\mathbf{k}}\right| \tag{125}$$

The value of $\mathrm{Tr}\left(\exp\left(-\beta\omega_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}\right)\right)$ is:

$$\mathrm{Tr}\left(\exp\left(-\beta\omega_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}\right)\right) = \mathrm{Tr}\left(\sum_{j}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|\right) \tag{126}$$

$$= \sum_{j}\exp\left(-j\beta\omega_{\mathbf{k}}\right) \tag{127}$$

$$= \sum_{j}\exp\left(-\beta\omega_{\mathbf{k}}\right)^{j} \tag{128}$$

$$= \frac{1}{1-\exp\left(-\beta\omega_{\mathbf{k}}\right)} \quad \text{(by geometric series)} \tag{129}$$

$$\equiv f_{\mathrm{Bose-Einstein}}\left(-\beta\omega_{\mathbf{k}}\right) \tag{130}$$

$$\mathrm{Tr}\left(\exp\left(-\beta\sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}\right)\right) = \mathrm{Tr}\left(\prod_{k}\sum_{j}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|\right) \tag{131}$$

$$= \prod_{k}\mathrm{Tr}\left(\sum_{j}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|\right) \tag{132}$$

$$= \prod_{k}f_{\mathrm{Bose-Einstein}}\left(-\beta\omega_{\mathbf{k}}\right) \tag{133}$$

So the density matrix of the bath is:

$$\rho_{B} = \frac{e^{-\beta H_{B}}}{\mathrm{Tr}\left(e^{-\beta H_{B}}\right)} \tag{134}$$

$$= \frac{\prod_{k}\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|}{\prod_{k}f_{\mathrm{Bose-Einstein}}\left(-\beta\omega_{\mathbf{k}}\right)} \tag{135}$$

$$= \prod_{k}\frac{\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|}{f_{\mathrm{Bose-Einstein}}\left(-\beta\omega_{\mathbf{k}}\right)} \tag{136}$$

Now, given that creation and annihilation satisfy:

$$b_{\mathbf{k}}\,|\,j_{\mathbf{k}}\rangle = \sqrt{j_{\mathbf{k}}}\,|j_{\mathbf{k}}-1\rangle \tag{137}$$

$$b_{\mathbf{k}}^{\dagger}\,|\,j_{\mathbf{k}}\rangle = \sqrt{j_{\mathbf{k}}+1}\,|\,j_{\mathbf{k}}+1\rangle \tag{138}$$

Then we can prove that $\langle B_{z}\rangle_{H_{B}} = 0$ using the following property based on (137)-(138):

$$\langle B_{z}\rangle_{H_{B}} = \mathrm{Tr}\left(\rho_{B}B_{z}\right) = \mathrm{Tr}\left(B_{z}\rho_{B}\right) \tag{139}$$

$$= \mathrm{Tr}\left(\sum_{\mathbf{k}}\left(g_{\mathbf{k}}-v_{\mathbf{k}}\right)\left(b_{\mathbf{k}}^{\dagger}+b_{\mathbf{k}}\right)\rho_{B}\right) \tag{140}$$

$$= \sum_{\mathbf{k}}\mathrm{Tr}\left(\left(g_{\mathbf{k}}-v_{\mathbf{k}}\right)\left(b_{\mathbf{k}}^{\dagger}+b_{\mathbf{k}}\right)\rho_{B}\right) \tag{141}$$

$$= \sum_{\mathbf{k}}\mathrm{Tr}\left(\left(g_{\mathbf{k}}-v_{\mathbf{k}}\right)\left(b_{\mathbf{k}}^{\dagger}+b_{\mathbf{k}}\right)\prod_{\mathbf{k}}\frac{\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|}{f_{\mathrm{Bose-Einstein}}\left(-\beta\omega_{\mathbf{k}}\right)}\right) \tag{142}$$

$$= \left(g_{\mathbf{k}}-v_{\mathbf{k}}\right)\sum_{\mathbf{k}}\mathrm{Tr}\left(\left(b_{\mathbf{k}}^{\dagger}+b_{\mathbf{k}}\right)\prod_{\mathbf{k}}\frac{\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|}{f_{\mathrm{Bose-Einstein}}\left(-\beta\omega_{\mathbf{k}}\right)}\right) \tag{143}$$

$$= \left(g_{\mathbf{k}}-v_{\mathbf{k}}\right)\sum_{\mathbf{k}}\left(\mathrm{Tr}\left(b_{\mathbf{k}}^{\dagger}\prod_{\mathbf{k}}\frac{\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|}{f_{\mathrm{Bose-Einstein}}\left(-\beta\omega_{\mathbf{k}}\right)}\right) + \mathrm{Tr}\left(b_{\mathbf{k}}\prod_{\mathbf{k}}\frac{\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|}{f_{\mathrm{Bose-Einstein}}\left(-\beta\omega_{\mathbf{k}}\right)}\right)\right) \tag{144}$$

$$\text{Tr}\left(b_{\mathbf{k}}^{\dagger}\prod_{\mathbf{k}}\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|\right)=\text{Tr}\left(\left(\prod_{\mathbf{k}}\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)\right)b_{\mathbf{k}}^{\dagger}|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|\right)\quad\text{(by cyclic permutivity of trace, move }b_{\mathbf{k}}^{\dagger})\tag{145}$$

$$=\text{Tr}\left(\left(\prod_{\mathbf{k}}\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)\right)\sqrt{j_{\mathbf{k}}+1}\,|j_{\mathbf{k}}+1\rangle\langle j_{\mathbf{k}}|\right)\tag{146}$$

$$=0\tag{147}$$

$$\text{Tr}\left(b_{\mathbf{k}}\prod_{\mathbf{k}}\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|\right)=\text{Tr}\left(\left(\prod_{\mathbf{k}}\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)\right)b_{\mathbf{k}}|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|\right)\quad\text{(by cyclic permutivity of trace, move }b_{\mathbf{k}})\tag{148}$$

$$=\text{Tr}\left(\left(\prod_{\mathbf{k}}\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)\right)\sqrt{j_{\mathbf{k}}}\,|j_{\mathbf{k}}-1\rangle\langle j_{\mathbf{k}}|\right)\tag{149}$$

$$=0\tag{150}$$

we therefore find that:

$$\langle B_{z}\rangle_{H_{B}}=0\tag{151}$$

Another important expected value is $\langle B_{\pm}\rangle_{H_{B}}$, it's given by:

$$\langle B_{\pm}\rangle_{H_{B}}=\text{Tr}\left(\rho_{B}B_{\pm}\right)=\text{Tr}\left(B_{\pm}\rho_{B}\right)\tag{152}$$

$$=\text{Tr}\left(e^{\pm\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\left(b_{\mathbf{k}}^{\dagger}-b_{\mathbf{k}}\right)}\rho_{B}\right)\tag{153}$$

$$=\text{Tr}\left(e^{\pm\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\left(b_{\mathbf{k}}^{\dagger}-b_{\mathbf{k}}\right)}\prod_{k}\frac{\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|}{f_{\text{Bose}-\text{Einstein}}\left(-\beta\omega_{\mathbf{k}}\right)}\right)\tag{154}$$

$$=\text{Tr}\left(\left(\prod_{k}\frac{\sum_{j_{\mathbf{k}}}\exp\left(-j_{\mathbf{k}}\beta\omega_{\mathbf{k}}\right)|j_{\mathbf{k}}\rangle\langle j_{\mathbf{k}}|}{f_{\text{Bose}-\text{Einstein}}\left(-\beta\omega_{\mathbf{k}}\right)}\right)e^{\pm\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\left(b_{\mathbf{k}}^{\dagger}-b_{\mathbf{k}}\right)}\right)\tag{155}$$

$$=\tag{156}$$

$$=\exp\left(-(1/2)\sum_{\mathbf{k}}|\alpha_{\mathbf{k}}|^{2}\coth\left(\beta\omega_{\mathbf{k}}/2\right)\right)\tag{157}$$

$$\equiv B\tag{158}$$

Using the integral representation we could obtain that:the expected value for the displacement operator $D\left(h\right)$ with $h\in\mathbb{C}$ is equal to:

$$\langle D\left(h\right)\rangle = \frac{1}{\pi N}\int \exp\left(-\frac{|\alpha|^2}{N}\right)\langle\alpha|D\left(h\right)|\alpha\rangle\mathrm{d}^2\alpha \tag{159}$$

$$= \frac{1}{\pi N}\int \exp\left(-\frac{|\alpha|^2}{N}\right)\langle 0|D\left(-\alpha\right)D\left(h\right)D\left(\alpha\right)|0\rangle\mathrm{d}^2\alpha \tag{160}$$

$$D\left(h\right)D\left(\alpha\right) = D\left(h+\alpha\right)e^{\frac{1}{2}\left(h\alpha^*-h^*\alpha\right)} \tag{161}$$

$$D\left(-\alpha\right)\left(D\left(h\right)D\left(\alpha\right)\right) = D\left(-\alpha\right)D\left(h+\alpha\right)e^{\frac{1}{2}\left(h\alpha^*-h^*\alpha\right)} \tag{162}$$

$$= D\left(h\right)e^{\frac{1}{2}\left(-\alpha(h+\alpha)^*+\alpha^*(h+\alpha)\right)}e^{\frac{1}{2}\left(h\alpha^*-h^*\alpha\right)} \tag{163}$$

$$= D\left(\alpha\right)e^{\frac{1}{2}\left(-\alpha h^*-|\alpha|^2+\alpha^*h+|\alpha|^2\right)}e^{\frac{1}{2}\left(h\alpha^*-h^*\alpha\right)} \tag{164}$$

$$= D\left(\alpha\right)e^{\left(h\alpha^*-h^*\alpha\right)} \tag{165}$$

$$\langle D\left(h\right)\rangle = \frac{1}{\pi N}\int \exp\left(-\frac{|\alpha|^2}{N}\right)\langle 0|D\left(h\right)\exp\left(h\alpha^*-h^*\alpha\right)|0\rangle\mathrm{d}^2\alpha \tag{166}$$

$$= \frac{1}{\pi N}\int \exp\left(-\frac{|\alpha|^2}{N}\right)\exp\left(h\alpha^*-h^*\alpha\right)\langle 0|D\left(h\right)|0\rangle\mathrm{d}^2\alpha \tag{167}$$

$$= \frac{1}{\pi N}\int \exp\left(-\frac{|\alpha|^2}{N}\right)\exp\left(h\alpha^*-h^*\alpha\right)\langle 0|h\rangle\mathrm{d}^2\alpha \tag{168}$$

$$|\alpha\rangle = \exp\left(-\frac{|\alpha|^2}{2}\right)\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle \tag{169}$$

$$\langle D\left(h\right)\rangle = \frac{1}{\pi N}\int \exp\left(-\frac{|\alpha|^2}{N}\right)\exp\left(h\alpha^*-h^*\alpha\right)\langle 0|\exp\left(-\frac{|h|^2}{2}\right)\sum_{n=0}^{\infty}\frac{h^n}{\sqrt{n!}}|n\rangle\mathrm{d}^2\alpha \tag{170}$$

$$= \frac{1}{\pi N}\int \exp\left(-\frac{|\alpha|^2}{N}\right)\exp\left(h\alpha^*-h^*\alpha\right)\exp\left(-\frac{|h|^2}{2}\right)\mathrm{d}^2\alpha \tag{171}$$

$$= \frac{\exp\left(-\frac{|h|^2}{2}\right)}{\pi N}\int \exp\left(-\frac{|\alpha|^2}{N}+h\alpha^*-h^*\alpha\right)\mathrm{d}^2\alpha \tag{172}$$

$$\alpha = x+\mathrm{i}y \tag{173}$$

$$\langle D\left(h\right)\rangle = \frac{\exp\left(-\frac{|h|^2}{2}\right)}{\pi N}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp\left(-\frac{x^2+y^2}{N}+h\left(x-\mathrm{i}y\right)-h^*\left(x+\mathrm{i}y\right)\right)\mathrm{d}x\mathrm{d}y \tag{174}$$

$$= \frac{\exp\left(-\frac{|h|^2}{2}\right)}{\pi N}\int_{-\infty}^{\infty}\exp\left(-\frac{x^2}{N}+hx-h^*x\right)\mathrm{d}x\int_{-\infty}^{\infty}\exp\left(-\frac{y^2}{N}-\mathrm{i}hy-\mathrm{i}h^*y\right)\mathrm{d}y \tag{175}$$

$$-\frac{x^2}{N}+hx-h^*x = -\frac{1}{N}\left(x^2-Nhx+Nh^*x\right) \tag{176}$$

$$= -\frac{1}{N}\left(x+\frac{\left(Nh^*-Nh\right)}{2}\right)^2+\frac{N\left(h^*-h\right)^2}{4} \tag{177}$$

$$-\frac{y^2}{N}-\mathrm{i}hy-\mathrm{i}h^*y = -\frac{1}{N}\left(y^2+\mathrm{i}Nhy+\mathrm{i}Nh^*y\right) \tag{178}$$

$$= -\frac{1}{N}\left(y^2+\frac{\mathrm{i}N\left(h+h^*\right)}{2}\right)-\frac{N\left(h+h^*\right)^2}{4} \tag{179}$$

$$\langle D\left(h\right)\rangle = \frac{\exp\left(-\frac{|h|^2}{2} + \frac{N(h^*-h)^2}{4} - \frac{N(h+h^*)^2}{4}\right)}{\pi N} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp\left(-\frac{1}{N}\left(x + \frac{(Nh^*-Nh)}{2}\right)^2 - \frac{1}{N}\left(y^2 + \frac{iN\left(h+h^*\right)}{2}\right)\right)\mathrm{d}x\mathrm{d}y$$

(180)

$$\sqrt{2\pi}\sigma = \int_{-\infty}^{\infty}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)\mathrm{d}x$$

(181)

$$\langle D\left(h\right)\rangle = \frac{\exp\left(-\frac{|h|^2}{2} + \frac{N(h^*-h)^2}{4} - \frac{N(h+h^*)^2}{4}\right)}{\pi N} \int_{-\infty}^{\infty}\exp\left(-\frac{\left(x + \frac{(Nh^*-Nh)}{2}\right)^2}{2\left(\sqrt{\frac{N}{2}}\right)^2}\right)\mathrm{d}x \int_{-\infty}^{\infty}\exp\left(-\frac{\left(y^2 + \frac{iN(h+h^*)}{2}\right)}{2\left(\sqrt{\frac{N}{2}}\right)^2}\right)\mathrm{d}y$$

(182)

$$= \frac{\exp\left(-\frac{|h|^2}{2} + \frac{N(h^*-h)^2}{4} - \frac{N(h+h^*)^2}{4}\right)}{\pi N}\left(\sqrt{2\pi}\sqrt{\frac{N}{2}}\right)^2$$

(183)

$$= \exp\left(-\frac{|h|^2}{2} + \frac{N\left(h^* - h\right)^2}{4} - \frac{N\left(h+h^*\right)^2}{4}\right)$$

(184)

$$= \exp\left(-\frac{|h|^2}{2} + \frac{N\left(h^{*2} - 2hh^* + h^2\right) - N\left(h^2 + 2hh^* + h^{*2}\right)}{4}\right)$$

(185)

$$= \exp\left(-|h|^2\left(N + \frac{1}{2}\right)\right)$$

(186)

$$= \exp\left(-|h|^2\left(\frac{1}{e^{\beta\omega} - 1} + \frac{1}{2}\right)\right)$$

(187)

$$= \exp\left(-\frac{|h|^2}{2}\left(\frac{e^{\beta\omega} + 1}{e^{\beta\omega} - 1}\right)\right)$$

(188)

$$= \exp\left(-\frac{|h|^2}{2}\coth\left(\frac{\beta\omega}{2}\right)\right)$$

(189)

In the last line we used $\frac{e^{\beta\omega}+1}{e^{\beta\omega}-1} = \coth\left(\frac{\beta\omega}{2}\right)$. We will now force $\left\langle\overline{H_{\bar{I}}}\right\rangle_{H_B} = 0$. We will also introduce the bath renormalizing driving in $\overline{H_S}$ to treat it non-perturbatively in the subsequent formalism, we associate the terms related with $B_+\sigma_+$ and $B_-\sigma_-$ with the interaction part of the Hamiltonian $\overline{H_I}$ and we subtract their expected value in order to satisfy $\left\langle\overline{H_I}\right\rangle_{H_B} = 0$, furthermore we add the subtracted terms to the $\overline{H_S}$.

A final form of the terms of the splitted Hamiltonian $\overline{H}$ is:

$$\overline{H(t)} = \varepsilon_0\left(t\right)|0\rangle\langle 0| + \varepsilon_1\left(t\right)|1\rangle\langle 1| + V_{10}\left(t\right)|1\rangle\langle 0|B_{1+}B_{0-} + V_{01}\left(t\right)|0\rangle\langle 1|B_{0+}B_{1-} + \sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}}$$

(190)

$$+ \sum_{\mathbf{k}}\left(|0\rangle\langle 0|\left((g_{0\mathbf{k}} - \omega_{\mathbf{k}}\alpha_{0\mathbf{k}})b_{\mathbf{k}}^\dagger + (g_{0\mathbf{k}} - \omega_{\mathbf{k}}\alpha_{0\mathbf{k}})^* b_{\mathbf{k}}\right) + |1\rangle\langle 1|\left((g_{1\mathbf{k}} - \omega_{\mathbf{k}}\alpha_{1\mathbf{k}})b_{\mathbf{k}}^\dagger + (g_{1\mathbf{k}} - \omega_{\mathbf{k}}\alpha_{1\mathbf{k}})^* b_{\mathbf{k}}\right)\right)$$

(191)

$$+ \sum_{\mathbf{k}}\left(|0\rangle\langle 0|\left(\omega_{\mathbf{k}}|\alpha_{0\mathbf{k}}|^2 - (g_{0\mathbf{k}}\alpha_{0\mathbf{k}}^* + g_{0\mathbf{k}}^*\alpha_{0\mathbf{k}})\right) + |1\rangle\langle 1|\left(\omega_{\mathbf{k}}|\alpha_{1\mathbf{k}}|^2 - (g_{1\mathbf{k}}\alpha_{1\mathbf{k}}^* + g_{1\mathbf{k}}^*\alpha_{1\mathbf{k}})\right)\right)$$

(192)

$$= \left(\varepsilon_0\left(t\right) + R_0\right)|0\rangle\langle 0| + \left(\varepsilon_1\left(t\right) + R_1\right)|1\rangle\langle 1| + V_{10}\left(t\right)|1\rangle\langle 0|B_{1+}B_{0-} + V_{01}\left(t\right)|0\rangle\langle 1|B_{0+}B_{1-}$$

(193)

$$+ \sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + |0\rangle\langle 0|B_{0z} + |1\rangle\langle 1|B_{1z}$$

(194)

$$\equiv \overline{H_{\bar{S}}(t)} + \overline{H_{\bar{I}}} + \overline{H_{\bar{B}}}$$

(195)

The parts of the Hamiltonian splitted are obtained using the following expected value:

$$\langle B_{1+} B_{0-} \rangle = B_{10} \tag{196}$$

$$= \left\langle \prod_{\mathbf{k}} D\left(\alpha_{1\mathbf{k}}\right) \prod_{\mathbf{k}} D\left(-\alpha_{0\mathbf{k}}\right) \right\rangle \tag{197}$$

$$= \left\langle \prod_{\mathbf{k}} \left(D\left(\alpha_{1\mathbf{k}}\right) D\left(-\alpha_{0\mathbf{k}}\right)\right) \right\rangle = \tag{198}$$

$$= \left\langle \prod_{\mathbf{k}} \left(D\left(\alpha_{1\mathbf{k}} - \alpha_{0\mathbf{k}}\right) e^{\frac{1}{2}\left(\alpha_{1\mathbf{k}}^* \alpha_{0\mathbf{k}} - \alpha_{1\mathbf{k}} \alpha_{0\mathbf{k}}^*\right)}\right) \right\rangle \tag{199}$$

$$= \prod_{\mathbf{k}} \langle D\left(\alpha_{1\mathbf{k}} - \alpha_{0\mathbf{k}}\right) \rangle e^{\frac{1}{2}\left(\alpha_{1\mathbf{k}}^* \alpha_{0\mathbf{k}} - \alpha_{1\mathbf{k}} \alpha_{0\mathbf{k}}^*\right)} \tag{200}$$

$$= \left(\prod_{\mathbf{k}} e^{\frac{1}{2}\left(\alpha_{1\mathbf{k}}^* \alpha_{0\mathbf{k}} - \alpha_{1\mathbf{k}} \alpha_{0\mathbf{k}}^*\right)}\right) \left(\exp\left(-\frac{1}{2} \sum_{\mathbf{k}} |\alpha_{1\mathbf{k}} - \alpha_{0\mathbf{k}}|^2 \coth\left(\frac{\beta\omega}{2}\right)\right)\right) \tag{201}$$

From the definition $B_{10}^* = \langle B_{0+} B_{1-} \rangle$. In the section related with the free energy minimization we will consider that $\alpha_{1\mathbf{k}}, \alpha_{0\mathbf{k}} \in \mathbb{R}$ for all $\mathbf{k}$ in order to optimize a lower bound of the free-energy and calculate the derivates.

$$\langle B_{1+} B_{0-} \rangle = \left(\exp\left(-\sum_{\mathbf{k}} \left(\alpha_{1\mathbf{k}} - \alpha_{0\mathbf{k}}\right)^2 \coth\left(\frac{\beta\omega}{2}\right)\right)\right) \tag{202}$$

The parts of the Hamiltonian splitted are:

$$\overline{H_{\bar{S}}(t)} \equiv \left(\varepsilon_0\left(t\right) + R_0\right) |0\rangle\langle 0| + \left(\varepsilon_1\left(t\right) + R_1\right) |1\rangle\langle 1| + V_{10}\left(t\right) B_{10}\sigma_+ + V_{01}\left(t\right) B_{10}\sigma_- \tag{203}$$

$$\overline{H_{\bar{I}}} \equiv V_{10}\left(t\right) \left(\sigma_+ B_{1+} B_{0-} - \sigma_+ B_{10}\right) + V_{01}\left(t\right) \left(\sigma_- B_{0+} B_{1-} - \sigma_- B_{10}\right) + |0\rangle\langle 0| B_{0z} + |1\rangle\langle 1| B_{1z} \tag{204}$$

$$\overline{H_{\bar{B}}} \equiv \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \tag{205}$$

$$= H_B \tag{206}$$

Note that $\overline{H_{\bar{B}}}$, which is the bath acting on the effective "system" $\bar{S}$ in the variational frame, is just the original bath, H_B, before transforming to the variational frame.

For the Hamiltonian (204) we can verify the condition $\left\langle \overline{H_{\bar{I}}} \right\rangle_{H_B} = 0$ in the following way:

$$\left\langle \overline{H_{\bar{I}}} \right\rangle_{H_B} = \left\langle \sum_{n\mathbf{k}} \left(\left(g_{n\mathbf{k}} - v_{n\mathbf{k}}\right) b_{\mathbf{k}}^\dagger + \left(g_{n\mathbf{k}} - v_{n\mathbf{k}}\right)^* b_{\mathbf{k}}\right) |n\rangle\langle n| + V_{10}\left(t\right) \left(\sigma_+ B_{1+} B_{0-} - \sigma_+ B_{10}\right) + V_{01}\left(t\right) \left(\sigma_- B_{0+} B_{1-} - \sigma_- B_{10}^*\right) \right\rangle_{H_B} \tag{207}$$

$$= \left\langle \sum_{n\mathbf{k}} \left(\left(g_{n\mathbf{k}} - v_{n\mathbf{k}}\right) b_{\mathbf{k}}^\dagger + \left(g_{n\mathbf{k}} - v_{n\mathbf{k}}\right)^* b_{\mathbf{k}}\right) |n\rangle\langle n| \right\rangle_{H_B} + \langle V_{10}\left(t\right) \sigma_+ B_{1+} B_{0-} \rangle_{H_B} - \langle V_{10}\left(t\right) \sigma_+ B_{10} \rangle_{H_B} \tag{208}$$

$$+ \langle V_{01}\left(t\right) \sigma_- B_{0+} B_{1-} \rangle_{H_B} - \langle V_{01}\left(t\right) \sigma_- B_{10}^* \rangle_{H_B} \tag{209}$$

$$= \sum_{n\mathbf{k}} \left(\left\langle \left(g_{n\mathbf{k}} - v_{n\mathbf{k}}\right) b_{\mathbf{k}}^\dagger \right\rangle_{H_B} + \left\langle \left(g_{n\mathbf{k}} - v_{n\mathbf{k}}\right)^* b_{\mathbf{k}} \right\rangle_{H_B}\right) |n\rangle\langle n| + V_{10}\left(t\right) \sigma_+ \langle B_{1+} B_{0-} \rangle_{H_B} - V_{10}\left(t\right) \sigma_+ \langle B_{10} \rangle_{H_B} \tag{210}$$

$$= + V_{01}\left(t\right) \sigma_- \langle B_{0+} B_{1-} \rangle_{H_B} - V_{01}\left(t\right) \sigma_- \langle B_{10}^* \rangle_{H_B} \tag{211}$$

$$= \sum_{n\mathbf{k}} \left(\left(g_{n\mathbf{k}} - v_{n\mathbf{k}}\right) \left\langle b_{\mathbf{k}}^\dagger \right\rangle_{H_B} + \left(g_{n\mathbf{k}} - v_{n\mathbf{k}}\right)^* \langle b_{\mathbf{k}} \rangle_{H_B}\right) |n\rangle\langle n| + V_{10}\left(t\right) \sigma_+ \langle B_{1+} B_{0-} \rangle_{H_B} - V_{10}\left(t\right) \sigma_+ B_{10} \tag{212}$$

$$+ V_{01}\left(t\right) \sigma_- \langle B_{0+} B_{1-} \rangle_{H_B} - V_{01}\left(t\right) \sigma_- B_{10}^* \tag{213}$$

$$= \sum_{n\mathbf{k}} \left(\left(g_{n\mathbf{k}} - v_{n\mathbf{k}}\right) \left\langle b_{\mathbf{k}}^\dagger \right\rangle_{H_B} + \left(g_{n\mathbf{k}} - v_{n\mathbf{k}}\right)^* \langle b_{\mathbf{k}} \rangle_{H_B}\right) |n\rangle\langle n| + V_{10}\left(t\right) \sigma_+ B_{10} - V_{10}\left(t\right) \sigma_+ B_{10} \tag{214}$$

$$+ V_{01}\left(t\right) \sigma_- B_{10}^* - V_{01}\left(t\right) \sigma_- B_{10}^* \tag{215}$$

$$= 0 \tag{216}$$

We used (151) and (152) to evaluate the expected values.

Let's consider the following Hermitian combinations:

$$B_x = B_x^\dagger \tag{217}$$

$$= \frac{B_{1+}B_{0-} + B_{0+}B_{1-} - 2B_{10}}{2} \tag{218}$$

$$B_y = B_y^\dagger \tag{219}$$

$$= \frac{B_{0+}B_{1-} - B_{1+}B_{0-}}{2i} \tag{220}$$

$$B_{iz} = B_{iz}^\dagger \tag{221}$$

$$= \sum_{\mathbf{k}} \left((g_{i\mathbf{k}} - v_{i\mathbf{k}}) b_{\mathbf{k}}^\dagger + (g_{i\mathbf{k}} - v_{i\mathbf{k}})^* b_{\mathbf{k}} \right) \tag{222}$$

Writing the equations (203) and (204) using the previous combinations we obtain that:

$V_{10}(t)(\sigma_+ B_{1+}B_{0-} - \sigma_+ B_{10}) + V_{01}(t)(\sigma_- B_{0+}B_{1-} - \sigma_- B_{10}) + |0\rangle\langle0|B_{0z} + |1\rangle\langle1|B_{1z}$

$$\overline{H_{\bar{S}}(t)} = (\varepsilon_0(t) + R_0)|0\rangle\langle0| + (\varepsilon_1(t) + R_1)|1\rangle\langle1| + V_{10}(t)B_{10}\sigma_+ + V_{01}(t)B_{10}\sigma_- \tag{223}$$

$$= (\varepsilon_0(t) + R_0)|0\rangle\langle0| + (\varepsilon_1(t) + R_1)|1\rangle\langle1| + V_{10}(t)B_{10}\frac{\sigma_x + i\sigma_y}{2} + V_{01}(t)B_{10}\frac{\sigma_x - i\sigma_y}{2} \tag{224}$$

$$= (\varepsilon_0(t) + R_0)|0\rangle\langle0| + (\varepsilon_1(t) + R_1)|1\rangle\langle1| + \frac{B_{10}\sigma_x}{2}(V_{10}(t) + V_{01}(t)) + \frac{iB_{10}\sigma_y}{2}(V_{10}(t) - V_{01}(t)) \tag{225}$$

$$\overline{H_{\bar{I}}} = V_{10}(t)(\sigma_+ B_{1+}B_{0-} - \sigma_+ B_{10}) + V_{01}(t)(\sigma_- B_{0+}B_{1-} - \sigma_- B_{10}) + |0\rangle\langle0|B_{0z} + |1\rangle\langle1|B_{1z} \tag{226}$$

$$= |0\rangle\langle0|B_{0z} + |1\rangle\langle1|B_{1z} + (\Re(V_{10}(t)) + i\Im(V_{10}(t)))(\sigma_+ B_{1+}B_{0-} - \sigma_+ B_{10}) \tag{227}$$

$$+ (\Re(V_{10}(t)) - i\Im(V_{10}(t)))(\sigma_- B_{0+}B_{1-} - \sigma_- B_{10}) \tag{228}$$

$$= \sum_i B_{iz}|i\rangle\langle i| + \Re(V_{10}(t))(\sigma_+ B_{1+}B_{0-} - \sigma_+ B_{10} + \sigma_- B_{0+}B_{1-} - \sigma_- B_{10}) \tag{229}$$

$$+ i\Im(V_{10}(t))(\sigma_+ B_{1+}B_{0-} - \sigma_+ B_{10} - \sigma_- B_{0+}B_{1-} + \sigma_- B_{10}) \tag{230}$$

$$= \sum_i B_{iz}|i\rangle\langle i| + \Re(V_{10}(t))\left(\frac{\sigma_x + i\sigma_y}{2}B_{1+}B_{0-} - \frac{\sigma_x + i\sigma_y}{2}B_{10} + \frac{\sigma_x - i\sigma_y}{2}B_{0+}B_{1-} - \frac{\sigma_x - i\sigma_y}{2}B_{10}\right) \tag{231}$$

$$+ i\Im(V_{10}(t))\left(\frac{\sigma_x + i\sigma_y}{2}B_{1+}B_{0-} - \frac{\sigma_x + i\sigma_y}{2}B_{10} - \frac{\sigma_x - i\sigma_y}{2}B_{0+}B_{1-} + \frac{\sigma_x - i\sigma_y}{2}B_{10}\right) \tag{232}$$

$$= \sum_i B_{iz}|i\rangle\langle i| + \Re(V_{10}(t))\left(\sigma_x\frac{B_{1+}B_{0-} + B_{0+}B_{1-} - 2B_{10}}{2} + i\sigma_y\frac{B_{1+}B_{0-} - B_{0+}B_{1-}}{2}\right) \tag{233}$$

$$+ i\Im(V_{10}(t))\left(i\sigma_y\frac{B_{1+}B_{0-} + B_{0+}B_{1-} - 2B_{10}}{2} + \sigma_x\frac{B_{1+}B_{0-} - B_{0+}B_{1-}}{2}\right) \tag{234}$$

$$= B_z|1\rangle\langle1| + \Re(V_{10}(t))\left(\sigma_x\frac{B_{1+}B_{0-} + B_{0+}B_{1-} - 2B_{10}}{2} + i^2\sigma_y\frac{B_{1+}B_{0-} - B_{0+}B_{1-}}{2i}\right) \tag{235}$$

$$+ i\Im(V_{10}(t))\left(i\sigma_y\frac{B_{1+}B_{0-} + B_{0+}B_{1-} - 2B_{10}}{2} + i\sigma_x\frac{B_{1+}B_{0-} - B_{0+}B_{1-}}{2i}\right) \tag{236}$$

$$= B_z|1\rangle\langle1| + \Re(V_{10}(t))\left(\sigma_x\frac{B_{1+}B_{0-} + B_{0+}B_{1-} - 2B_{10}}{2} + \sigma_y\frac{B_{0+}B_{1-} - B_{1+}B_{0-}}{2i}\right) \tag{237}$$

$$+ i\Im(V_{10}(t))\left(i\sigma_y\frac{B_{1+}B_{0-} + B_{0+}B_{1-} - 2B_{10}}{2} - i\sigma_x\frac{B_{0+}B_{1-} - B_{1+}B_{0-}}{2i}\right) \tag{238}$$

$$= B_z|1\rangle\langle1| + \Re(V_{10}(t))(B_x\sigma_x + B_y\sigma_y) + i\Im(V_{10}(t))(iB_x\sigma_y - iB_y\sigma_x) \tag{239}$$

$$= B_z|1\rangle\langle1| + \Re(V_{10}(t))(B_x\sigma_x + B_y\sigma_y) - \Im(V_{10}(t))(B_x\sigma_y - B_y\sigma_x). \tag{240}$$

III. FREE-ENERGY MINIMIZATION

The true free energy A is bounded by the Bogoliubov inequality:

$$A \leq A_{\mathrm{B}} \equiv -\frac{1}{\beta} \ln \left(\mathrm{Tr} \left(e^{-\beta(\overline{H_{\bar{S}}(t)} + H_B)} \right) \right) + \langle \overline{H_{\bar{I}}} \rangle_{\overline{H_{\bar{S}}(t)} + H_B} + O \left(\langle \overline{H_{\bar{I}}^2} \rangle_{\overline{H_{\bar{S}}(t)} + H_B} \right) \tag{241}$$

We will optimize the set of variational parameters $\{v_{\mathbf{k}}\}$ in order to minimize A_{B} (i.e. to make it as close to the true free energy A as possible). Neglecting the higher order terms and using $\langle \overline{H_{\bar{I}}} \rangle_{\overline{H_{\bar{S}}(t)} + H_B} = 0$ we can obtain the following condition to obtain the set $\{v_{\mathbf{k}}\}$:

$$\frac{\partial A_{\mathrm{B}}}{\partial v_{\mathbf{k}}} = 0. \tag{242}$$

Using this condition and given that $\left[\overline{H_{\bar{S}}(t)}, H_B \right] = 0$, we have:

$$e^{-\beta\left(\overline{H_{\bar{S}}(t)} + H_B\right)} = e^{-\beta\overline{H_{\bar{S}}(t)}} e^{-\beta H_B} \tag{243}$$

Then using the fact that $\overline{H_{\bar{S}}(t)}$ and H_B relate to different Hilbert spaces, we obtain:

$$\mathrm{Tr} \left(e^{-\beta\overline{H_{\bar{S}}(t)}} e^{-\beta H_B} \right) = \mathrm{Tr} \left(e^{-\beta\overline{H_{\bar{S}}(t)}} \right) \mathrm{Tr} \left(e^{-\beta H_B} \right) \tag{244}$$

So Eq. (242) becomes:

$$\frac{\partial A_{\mathrm{B}}}{\partial v_{\mathbf{k}}} = -\frac{1}{\beta} \frac{\partial \ln \left(\mathrm{Tr} \left(e^{-\beta(\overline{H_{\bar{S}}(t)} + H_B)} \right) \right)}{\partial v_{\mathbf{k}}} \tag{245}$$

$$= -\frac{1}{\beta} \frac{\partial \ln \left(\mathrm{Tr} \left(e^{-\beta\overline{H_{\bar{S}}(t)}} \right) \mathrm{Tr} \left(e^{-\beta H_B} \right) \right)}{\partial v_{\mathbf{k}}} \tag{246}$$

$$= -\frac{1}{\beta} \frac{\partial \left(\ln \left(\mathrm{Tr} \left(e^{-\beta\overline{H_{\bar{S}}(t)}} \right) \right) + \ln \left(\mathrm{Tr} \left(e^{-\beta H_B} \right) \right) \right)}{\partial v_{\mathbf{k}}} \tag{247}$$

$$= -\frac{1}{\beta} \frac{\partial \ln \left(\mathrm{Tr} \left(e^{-\beta\overline{H_{\bar{S}}(t)}} \right) \right)}{\partial v_{\mathbf{k}}} - \frac{1}{\beta} \frac{\partial \ln \left(\mathrm{Tr} \left(e^{-\beta\overline{H_B}} \right) \right)}{\partial v_{\mathbf{k}}} \tag{248}$$

$$= 0 \quad \text{(by Eq. (242))}. \tag{249}$$

But since $\bar{H}_{\bar{B}} = H_B$ which doesn't contain any $v_{\mathbf{k}}$, a derivative of any function of H_B that does not introduce new $v_{\mathbf{k}}$ will be zero. We therefore require the following:

$$\frac{\partial \ln \left(\mathrm{Tr} \left(e^{-\beta\overline{H_{\bar{S}}(t)}} \right) \right)}{\partial v_{\mathbf{k}}} = \frac{1}{e^{-\beta\overline{H_{\bar{S}}(t)}}} \frac{\partial e^{-\beta\overline{H_{\bar{S}}(t)}}}{\partial v_{\mathbf{k}}} \tag{250}$$

$$= 0 \tag{251}$$

This means we need to impose:

$$\frac{\partial e^{-\beta\overline{H_{\bar{S}}(t)}}}{\partial v_{\mathbf{k}}} = 0 \tag{252}$$

First we look at:

$$-\beta\overline{H_{\bar{S}}(t)}(t) = -\beta \left((\varepsilon_0(t) + R_0) |0\rangle\langle 0| + (\varepsilon_1(t) + R_1) |1\rangle\langle 1| + V_{10}(t) B_{10} \sigma_+ + V_{01}(t) B_{10} \sigma_- \right). \tag{253}$$

Then the eigenvalues of $-\beta\overline{H_{\bar{S}}(t)}$ satisfy the following relationship deduced from the Caley-Hamilton theorem:

$$\lambda^2 - \text{Tr}\left(-\beta \overline{H_{\bar{S}}(t)}\right) + \text{Det}\left(-\beta \overline{H_{\bar{S}}(t)}\right) = 0 \tag{254}$$

Let's define:

$$\varepsilon(t) \equiv \text{Tr}\left(\overline{H_{\bar{S}}(t)}\right) \tag{255}$$

$$\eta \equiv \sqrt{\left(\text{Tr}\left(\overline{H_{\bar{S}}(t)}\right)\right)^2 - 4\text{Det}\left(\overline{H_{\bar{S}}(t)}\right)} \tag{256}$$

The solutions of the equation (254) are:

$$\lambda = \beta \frac{-\text{Tr}\left(\overline{H_{\bar{S}}(t)}\right) \pm \sqrt{\left(\text{Tr}\left(\overline{H_{\bar{S}}(t)}\right)\right)^2 - 4\text{Det}\left(\overline{H_{\bar{S}}(t)}\right)}}{2} \tag{257}$$

$$= \beta \frac{-\varepsilon(t) \pm \eta(t)}{2} \tag{258}$$

$$= -\beta \frac{\varepsilon(t) \mp \eta(t)}{2} \tag{259}$$

`tic; det(rand(10000)); toc;` in Matlab takes 6 seconds on Laptop, so determinant of the system is no problem. Though $\overline{H_{\bar{S}}(t)}$ has a B in it with depends on bath degrees of freedom. For this equation is it S or $\bar{S}$? (It's $\bar{S}$). Also this will have to be re-done for every time step, so it is indeed it is time consuming compared to for example: `tic; exp(rand(10000)); toc;`. Funny it turns out that `det(10000) = exp(trace(log(rand(10000))))`actually only takes 2 seconds instead of 6.

The value of $\text{Tr}\left(e^{-\beta \overline{H_{\bar{S}}(t)}}\right)$ can be written in terms of this eigenvalues as (since there's only 2 eigenvalues of a 2×2 matrix):

$$\text{Tr}\left(e^{-\beta \overline{H_{\bar{S}}(t)}}\right) = \exp\left(-\frac{\varepsilon(t)\beta}{2}\right)\exp\left(\frac{\eta(t)\beta}{2}\right) + \exp\left(-\frac{\varepsilon(t)\beta}{2}\right)\exp\left(-\frac{\eta(t)\beta}{2}\right) \tag{260}$$

$$= 2\exp\left(-\frac{\varepsilon(t)\beta}{2}\right)\cosh\left(\frac{\eta(t)\beta}{2}\right) \tag{261}$$

Using the chain rule on the function $\text{Tr}\left(e^{-\beta \overline{H_{\bar{S}}(t)}}\right) = A\left(\varepsilon(t), \eta(t)\right)$ to calculate $\frac{\partial \text{Tr}\left(e^{-\beta \overline{H_{\bar{S}}(t)}}\right)}{\partial v_{i\mathbf{k}}}$ can lead to calculate as intermediate step $\frac{\partial \text{Tr}\left(e^{-\beta \overline{H_{\bar{S}}(t)}}\right)}{\partial \alpha_{i\mathbf{k}}}$ because $\frac{\mathrm{d}\alpha_{i\mathbf{k}}}{\mathrm{d}v_{i\mathbf{k}}} \frac{\partial \text{Tr}\left(e^{-\beta \overline{H_{\bar{S}}(t)}}\right)}{\partial \alpha_{i\mathbf{k}}} = \frac{\partial \text{Tr}\left(e^{-\beta \overline{H_{\bar{S}}(t)}}\right)}{\partial v_{i\mathbf{k}}}$:

$$\frac{\partial \text{Tr}\left(e^{-\beta \overline{H_{\bar{S}}(t)}}\right)}{\partial \alpha_{i\mathbf{k}}} = \frac{\partial\left(2\exp\left(-\frac{\varepsilon(t)\beta}{2}\right)\cosh\left(\frac{\eta(t)\beta}{2}\right)\right)}{\partial \alpha_{i\mathbf{k}}} \tag{262}$$

$$= 2\left(-\frac{\beta}{2}\frac{\partial \varepsilon(t)}{\partial \alpha_{i\mathbf{k}}}\right)\exp\left(-\frac{\varepsilon(t)\beta}{2}\right)\cosh\left(\frac{\eta(t)\beta}{2}\right) + 2\left(\frac{\beta}{2}\frac{\partial \eta(t)}{\partial \alpha_{i\mathbf{k}}}\right)\exp\left(-\frac{\varepsilon(t)\beta}{2}\right)\sinh\left(\frac{\eta(t)\beta}{2}\right) \tag{263}$$

$$= -\beta\exp\left(-\frac{\varepsilon(t)\beta}{2}\right)\left(\frac{\partial \varepsilon(t)}{\partial \alpha_{i\mathbf{k}}}\cosh\left(\frac{\eta(t)\beta}{2}\right) - \frac{\partial \eta(t)}{\partial \alpha_{i\mathbf{k}}}\sinh\left(\frac{\eta(t)\beta}{2}\right)\right) \tag{264}$$

Making the derivate equal to zero make us suitable to write:

$$\frac{\partial \varepsilon(t)}{\partial \alpha_{i\mathbf{k}}}\cosh\left(\frac{\eta(t)\beta}{2}\right) - \frac{\partial \eta(t)}{\partial \alpha_{i\mathbf{k}}}\sinh\left(\frac{\eta(t)\beta}{2}\right) = 0 \tag{265}$$

The derivates included in the expression given are related to:

$$R_i = \sum_{\mathbf{k}}\left(\omega_{\mathbf{k}}|\alpha_{i\mathbf{k}}|^2 - (g_{i\mathbf{k}}\alpha_{i\mathbf{k}}^* + g_{i\mathbf{k}}^*\alpha_{i\mathbf{k}})\right), \ B_{10} = \left(\exp\left(-\frac{1}{2}\sum_{\mathbf{k}}(\alpha_{1\mathbf{k}} - \alpha_{0\mathbf{k}})^2\coth\left(\frac{\beta\omega}{2}\right)\right)\right): \tag{266}$$

$$\frac{\partial \varepsilon(t)}{\partial \alpha_{i\mathbf{k}}} = \frac{\partial\left(\varepsilon_1(t) + R_1 + \varepsilon_0(t) + R_0\right)}{\partial \alpha_{i\mathbf{k}}} \tag{267}$$

$$= \frac{\partial\left(\omega_{\mathbf{k}}|\alpha_{i\mathbf{k}}|^2 - \left(g_{i\mathbf{k}}\alpha_{i\mathbf{k}}^* + g_{i\mathbf{k}}^*\alpha_{i\mathbf{k}}\right)\right)}{\partial \alpha_{i\mathbf{k}}} = 2\omega_{\mathbf{k}}\alpha_{i\mathbf{k}} - \left(g_{i\mathbf{k}} + g_{i\mathbf{k}}^*\right) \tag{268}$$

$$\frac{\partial \eta(t)}{\partial \alpha_{i\mathbf{k}}} = \frac{\partial \sqrt{\left(\mathrm{Tr}\left(\overline{H_{\bar{S}}(t)}\right)\right)^2 - 4\mathrm{Det}\left(\overline{H_{\bar{S}}(t)}\right)}}{\partial \alpha_{i\mathbf{k}}} \tag{269}$$

$$= \frac{2\mathrm{Tr}\left(\overline{H_{\bar{S}}(t)}\right)\frac{\partial \mathrm{Tr}\left(\overline{H_{\bar{S}}(t)}\right)}{\partial \alpha_{i\mathbf{k}}} - 4\frac{\partial \mathrm{Det}\left(\overline{H_{\bar{S}}(t)}\right)}{\partial \alpha_{i\mathbf{k}}}}{2\sqrt{\left(\mathrm{Tr}\left(\overline{H_{\bar{S}}(t)}\right)\right)^2 - 4\mathrm{Det}\left(\overline{H_{\bar{S}}(t)}\right)}} \tag{270}$$

$$= \frac{\varepsilon(t)\left(2\omega_{\mathbf{k}}\alpha_{i\mathbf{k}} - \left(g_{i\mathbf{k}} + g_{i\mathbf{k}}^*\right)\right) - 2\frac{\partial\left((\varepsilon_1(t)+R_1)(\varepsilon_0(t)+R_0)-|V_{10}(t)|^2 B_{10}^2\right)}{\partial \alpha_{i\mathbf{k}}}}{\eta(t)} \tag{271}$$

$$= \frac{\varepsilon(t)\left(2\omega_{\mathbf{k}}\alpha_{i\mathbf{k}} - \left(g_{i\mathbf{k}} + g_{i\mathbf{k}}^*\right)\right) - 2\left(\left(\varepsilon(t) - \varepsilon_i(t) - R_i\right)\left(2\omega_{\mathbf{k}}\alpha_{i\mathbf{k}} - \left(g_{i\mathbf{k}} + g_{i\mathbf{k}}^*\right)\right) + 2|V_{10}(t)|^2 B_{10}^2\alpha_{i\mathbf{k}}\coth\left(\beta\omega_{\mathbf{k}}/2\right)\right)}{\eta(t)} \tag{272}$$

$$= \frac{\alpha_{i\mathbf{k}}}{\eta(t)}\left(2\omega_{\mathbf{k}}\varepsilon(t) - 4\left(\varepsilon(t) - \varepsilon_i(t) - R_i\right)\omega_{\mathbf{k}} - 4|V_{10}(t)|^2 B_{10}^2\coth\left(\beta\omega_{\mathbf{k}}/2\right)\right) \tag{273}$$

$$- \frac{\left(\left(g_{i\mathbf{k}} + g_{i\mathbf{k}}^*\right)\varepsilon(t) - 2\left(g_{i\mathbf{k}} + g_{i\mathbf{k}}^*\right)\left(\varepsilon(t) - \varepsilon_i(t) - R_i\right)\right)}{\eta(t)} \tag{274}$$

We made a simplification considering $\alpha_{\mathbf{k}} \in \mathbb{R}^+$ in order to be able to derivate because in general the derivate $\frac{\partial \overline{\alpha_{\mathbf{k}}}}{\partial \alpha_{\mathbf{k}}}$, $\frac{\partial |\alpha_{\mathbf{k}}|}{\partial \alpha_{\mathbf{k}}}$ are not well defined if $\alpha_{\mathbf{k}} \notin \mathbb{R}$. From the equation (265) and replacing the derivates obtained we have:

$$\tanh\left(\frac{\beta\eta(t)}{2}\right) = \frac{\frac{\partial \varepsilon(t)}{\partial \alpha_{i\mathbf{k}}}}{\frac{\partial \eta(t)}{\partial \alpha_{i\mathbf{k}}}} \tag{275}$$

$$= \frac{2\omega_{\mathbf{k}}\alpha_{i\mathbf{k}} - \left(g_{i\mathbf{k}} + g_{i\mathbf{k}}^*\right)}{\frac{\alpha_{i\mathbf{k}}\left(2\omega_{\mathbf{k}}\varepsilon(t)-4(\varepsilon(t)-\varepsilon_i(t)-R_i)\omega_{\mathbf{k}}-4|V_{10}(t)|^2 B_{10}^2\coth(\beta\omega_{\mathbf{k}}/2)\right)-\left(\left(g_{i\mathbf{k}}+g_{i\mathbf{k}}^*\right)\varepsilon(t)-2\left(g_{i\mathbf{k}}+g_{i\mathbf{k}}^*\right)(\varepsilon(t)-\varepsilon_i(t)-R_i)\right)}{\eta(t)}} \tag{276}$$

Rearrannging this equation and using $\alpha_{i\mathbf{k}} = \frac{v_{i\mathbf{k}}}{\omega_{i\mathbf{k}}}$ will lead to:

$$\tanh\left(\frac{\beta\eta(t)}{2}\right) = \frac{\left(2\omega_{\mathbf{k}}\frac{v_{i\mathbf{k}}}{\omega_{\mathbf{k}}} - \left(g_{i\mathbf{k}} + g_{i\mathbf{k}}^*\right)\right)\eta(t)}{\frac{v_{i\mathbf{k}}}{\omega_{\mathbf{k}}}\omega_{\mathbf{k}}\left(2\varepsilon(t)-4(\varepsilon(t)-\varepsilon_i(t)-R_i)-\frac{4|V_{10}(t)|^2 B_{10}^2\coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}}\right) - \left(g_{i\mathbf{k}}+g_{i\mathbf{k}}^*\right)(\varepsilon(t)-2(\varepsilon(t)-\varepsilon_i(t)-R_i))} \tag{277}$$

$$= \frac{\left(2v_{i\mathbf{k}} - \left(g_{i\mathbf{k}} + g_{i\mathbf{k}}^*\right)\right)\eta(t)}{v_{i\mathbf{k}}\left(2\varepsilon(t)-4(\varepsilon(t)-\varepsilon_i(t)-R_i)-\frac{4|V_{10}(t)|^2 B_{10}^2\coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}}\right) - \left(g_{i\mathbf{k}}+g_{i\mathbf{k}}^*\right)(\varepsilon(t)-2(\varepsilon(t)-\varepsilon_i(t)-R_i))} \tag{278}$$

$$= \frac{\left(2v_{i\mathbf{k}} - \left(g_{i\mathbf{k}} + g_{i\mathbf{k}}^*\right)\right)\eta(t)}{v_{i\mathbf{k}}\left(2\varepsilon(t)-4(\varepsilon(t)-\varepsilon_i(t)-R_i)-\frac{4|V_{10}(t)|^2 B_{10}^2\coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}}\right) - \left(g_{i\mathbf{k}}+g_{i\mathbf{k}}^*\right)(2\varepsilon_i(t)+2R_i-\varepsilon(t))} \tag{279}$$

Separating (279) such that the terms with $v_{\mathbf{k}}$ are located at one side of the equation permit us to write

$$2\frac{\eta\left(t\right)}{\tanh\left(\frac{\beta\eta(t)}{2}\right)}\left(v_{i\mathbf{k}}-\Re\left(g_{i\mathbf{k}}\right)\right)=2v_{i\mathbf{k}}\left(\varepsilon\left(t\right)-2\left(\varepsilon\left(t\right)-\varepsilon_{i}\left(t\right)-R_{i}\right)-\frac{2|V_{10}\left(t\right)|^{2}B_{10}^{2}\coth\left(\beta\omega_{\mathbf{k}}/2\right)}{\omega_{\mathbf{k}}}\right)$$
(280)

$$-\,2\Re\left(g_{i\mathbf{k}}\right)\left(2\varepsilon_{i}\left(t\right)+2R_{i}-\varepsilon\left(t\right)\right)$$
(281)

$$\frac{\eta\left(t\right)}{\tanh\left(\frac{\beta\eta(t)}{2}\right)}\left(v_{i\mathbf{k}}-\Re\left(g_{i\mathbf{k}}\right)\right)=v_{i\mathbf{k}}\left(\varepsilon\left(t\right)-2\left(\varepsilon\left(t\right)-\varepsilon_{i}\left(t\right)-R_{i}\right)-\frac{2|V_{10}\left(t\right)|^{2}B_{10}^{2}\coth\left(\beta\omega_{\mathbf{k}}/2\right)}{\omega_{\mathbf{k}}}\right)$$
(282)

$$-\,\Re\left(g_{\mathbf{k}}\right)\left(2\varepsilon_{i}\left(t\right)+2R_{i}-\varepsilon\left(t\right)\right)$$
(283)

$$\Re\left(g_{i\mathbf{k}}\right)\left(1-2\left(\varepsilon_{i}\left(t\right)+R_{i}-\frac{\varepsilon\left(t\right)}{2}\right)\frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta\left(t\right)}\right)=v_{i\mathbf{k}}\left(1-\frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta\left(t\right)}\left(\varepsilon\left(t\right)-2\left(\varepsilon\left(t\right)-\varepsilon_{i}\left(t\right)-R_{i}\right)\right.\right.$$
(284)

$$\left.\left.-\frac{2|V_{10}\left(t\right)|^{2}B_{10}^{2}\coth\left(\beta\omega_{\mathbf{k}}/2\right)}{\omega_{\mathbf{k}}}\right)\right)$$
(285)

The variational parameters are:

$$v_{i\mathbf{k}}=\frac{\Re\left(g_{i\mathbf{k}}\right)\left(1-\left(2\varepsilon_{i}\left(t\right)+2R_{i}-\varepsilon\left(t\right)\right)\frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)}\right)}{\left(1-\frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)}\left(\varepsilon\left(t\right)-2\left(\varepsilon\left(t\right)-\varepsilon_{i}\left(t\right)-R_{i}\right)-\frac{2|V_{10}(t)|^{2}B_{10}^{2}\coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}}\right)\right)}$$
(286)

IV. MASTER EQUATION

In order to describe the dynamics of the QD under the influence of the phonon environment, we use the time-convolutionless projection operator technique. We consider the QD in its ground state. The initial density operator $\rho_{\text{Total}}\left(0\right)=\rho_{S}(0)\otimes\rho_{B}^{\text{Thermal}}$, the transformed density operator is equal to:

$$\overline{\rho_{T}(0)}\equiv e^{V}\rho_{T}\left(0\right)e^{-V}$$
(287)

$$=\left(|0\rangle\langle0|+|1\rangle\langle1|B_{+}\right)\left(\rho_{S}(0)\otimes\rho_{B}^{\text{Thermal}}\right)\left(|0\rangle\langle0|+|1\rangle\langle1|B_{-}\right)$$
(288)

$$\text{for }\rho_{S}(0)=|0\rangle\langle0|:=|0\rangle\langle0|0\rangle\langle0|\rho_{B}^{\text{Thermal}}|0\rangle\langle0|$$
(289)

$$=|0\rangle\langle0|\otimes\rho_{B}^{\text{Thermal}}$$
(290)

$$=\rho_{T}\left(0\right)$$
(291)

$$\text{for }\rho_{S}(0)=|1\rangle\langle1|:=|1\rangle\langle1|B_{+}|1\rangle\langle1|\rho_{B}^{\text{Thermal}}|1\rangle\langle1|B_{-}$$
(292)

$$=|1\rangle\langle1|B_{+}\rho_{B}^{\text{Thermal}}B_{-}$$
(293)

$$=|1\rangle\langle1|\otimes B_{+}\rho_{B}^{\text{Thermal}}B_{-}$$
(294)

$$\text{for }\rho_{S}(0)=|0\rangle\langle1|:=|0\rangle\langle0|0\rangle\langle1|\rho_{B}^{\text{Thermal}}|1\rangle\langle1|B_{-}$$
(295)

$$=|0\rangle\langle1|\rho_{B}^{\text{Thermal}}|1\rangle\langle1|B_{-}$$
(296)

$$=|0\rangle\langle1|1\rangle\langle1|\rho_{B}^{\text{Thermal}}B_{-}$$
(297)

$$=|0\rangle\langle1|\otimes\rho_{B}^{\text{Thermal}}B_{-}$$
(298)

$$\text{for }\rho_{S}(0)=|1\rangle\langle0|:=|1\rangle\langle1|B_{+}|1\rangle\langle0|\rho_{B}^{\text{Thermal}}|0\rangle\langle0|$$
(299)

$$=|1\rangle\langle0|\otimes B_{+}\rho_{B}^{\text{Thermal}}$$
(300)

We transform any operator O into the interaction picture in the following way:

$$\widetilde{O}(t) \equiv U^{\dagger}(t) O(t) U(t) \tag{301}$$

$$U(t) \equiv \mathcal{T}\exp\left(-\mathrm{i}\int_0^t \mathrm{d}v \overline{H_{\tilde{S}}}(v)\right). \tag{302}$$

Therefore:

$$\widetilde{\overline{\rho_S}}(t) = U^{\dagger}(t)\overline{\rho_S}(t)U(t), \text{ where} \tag{303}$$

$$\overline{\rho_S}(t) = \mathrm{Tr}_B\left(\bar{\rho_T}(t)\right) \tag{304}$$

. In order to separate the Hamiltonian we define the matrix $\Lambda(t)$ such that $\Lambda_{1i}(t) = A_i$, $\Lambda_{2i}(t) = B_i$ and $\Lambda_{3i}(t) = C_i(t)$.

$$\Lambda(t) = \begin{pmatrix} \sigma_x & \sigma_y & \frac{I+\sigma_z}{2} & \sigma_x & \sigma_y & \frac{I-\sigma_z}{2} \\ B_x & B_y & B_{1z} & B_y & B_x & B_{2z} \\ \Re\left(V_{10}(t)\right) & \Re\left(V_{10}(t)\right) & 1 & \Im\left(V_{10}(t)\right) & -\Im\left(V_{10}(t)\right) & 1 \end{pmatrix} \tag{305}$$

In this case $|1\rangle\langle 1| = \frac{I+\sigma_z}{2}$ and $|0\rangle\langle 0| = \frac{I-\sigma_z}{2}$.

The previous notation allows us to write the interaction Hamiltonian $\overline{H_{\bar{I}}}(t)$ as pointed in the equation (236):

$$\overline{H_{\bar{I}}}(t) = B_{0z}|0\rangle\langle 0| + B_{1z}|1\rangle\langle 1| + \Re\left(V_{10}(t)\right)\left(B_x\sigma_x + B_y\sigma_y\right) - \Im\left(V_{10}(t)\right)\left(B_x\sigma_y - B_y\sigma_x\right) \tag{306}$$

$$= \Re\left(V_{10}(t)\right)\sigma_x B_x + \Re\left(V_{10}(t)\right)\sigma_y B_y + \frac{I+\sigma_z}{2}B_{1z} + \Im\left(V_{10}(t)\right)B_y\sigma_x - \Im\left(V_{10}(t)\right)B_x\sigma_y + \frac{I-\sigma_z}{2}B_{2z} \tag{307}$$

$$= \sum_i C_i(t)\left(A_i \otimes B_i(t)\right) \tag{308}$$

Taking as reference state ρ_B^{Thermal} and truncating at second order in $\overline{H_{\bar{I}}}(t)$, we obtain our master equation in the interaction picture:

$$\frac{\mathrm{d}\widetilde{\overline{\rho_S}}(t)}{\mathrm{d}t} = -\int_0^t \mathrm{Tr}_B\left[\widetilde{\overline{H_{\bar{I}}}}(t), \left[\widetilde{\overline{H_{\bar{I}}}}(s), \widetilde{\overline{\rho_S}}(t)\rho_B^{\text{Thermal}}\right]\right]\mathrm{d}s \tag{309}$$

From the interaction picture applied on $\overline{H_{\bar{I}}}(t)$ we find:

$$\widetilde{\overline{H_{\bar{I}}}}(t) = U^{\dagger}(t)\,\overline{H_{\bar{I}}}(t)\,U(t) \tag{310}$$

we use the time-ordering operator $\mathcal{T}$ because in general $\overline{H_{\tilde{S}}}(t)$ doesn't conmute with itself at two different times. We write the interaction Hamiltonian as:

$$\widetilde{\overline{H_{\bar{I}}}}(t) = \sum_i C_i(t)\left(\widetilde{A_i}(t) \otimes \widetilde{B_i}(t)\right) \tag{311}$$

$$\widetilde{A_i}(t) = U^{\dagger}(t) A_i U(t) \tag{312}$$

$$\widetilde{B_i}(t) = \mathrm{e}^{\mathrm{i}H_B t} B_i(t)\,\mathrm{e}^{-\mathrm{i}H_B t} \tag{313}$$

Using the expression (311) to replace it in the equation (309)

$$\frac{\mathrm{d}\widetilde{\widetilde{\rho_S}}(t)}{\mathrm{d}t} = -\int_0^t \mathrm{Tr}_B\left[\widetilde{\widetilde{H_I}}(t),\left[\widetilde{\widetilde{H_I}}(s),\widetilde{\widetilde{\rho_S}}(t)\rho_B^{\mathrm{Thermal}}\right]\right]\mathrm{d}s \tag{314}$$

$$= -\int_0^t \mathrm{Tr}_B\left[\sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right),\left[\sum_i C_i(s)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right),\widetilde{\widetilde{\rho_S}}(t)\rho_B^{\mathrm{Thermal}}\right]\right]\mathrm{d}s \tag{315}$$

$$= -\int_0^t \mathrm{Tr}_B\left[\sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right),\sum_i C_i(s)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\widetilde{\widetilde{\rho_S}}(t)\rho_B^{\mathrm{Thermal}} -\widetilde{\widetilde{\rho_S}}(t)\rho_B^{\mathrm{Thermal}}\sum_i C_i(s)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\right]\mathrm{d}s \tag{316}$$

$$= -\int_0^t \mathrm{Tr}_B\left(\sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right)\sum_i C_i(s)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\widetilde{\widetilde{\rho_S}}(t)\rho_B^{\mathrm{Thermal}} \right. \tag{317}$$

$$-\sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right)\widetilde{\widetilde{\rho_S}}(t)\rho_B^{\mathrm{Thermal}}\sum_i C_i(s)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right) \tag{318}$$

$$-\sum_{i\in J} C_i(s)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\widetilde{\widetilde{\rho_S}}(t)\rho_B^{\mathrm{Thermal}}\sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right) \tag{319}$$

$$\left.+\widetilde{\widetilde{\rho_S}}(t)\rho_B^{\mathrm{Thermal}}\sum_i C_i(s)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right)\right)\mathrm{d}s \tag{320}$$

In order to calculate the correlation functions we define:

$$\Lambda_{ji}(\tau) = \left\langle\widetilde{B_j}(t)\widetilde{B_i}(s)\right\rangle_B \tag{321}$$

$$= \left\langle\widetilde{B_j}(\tau)\widetilde{B_i}(0)\right\rangle_B \tag{322}$$

The correlation functions relevant that appear in the equation (314) are:

$$\mathrm{Tr}_B\left(\widetilde{B_j}(t)\widetilde{B_i}(s)\rho_B^{\mathrm{Thermal}}\right) = \left\langle\widetilde{B_j}(t)\widetilde{B_i}(s)\right\rangle_B \tag{323}$$

$$= \left\langle\widetilde{B_j}(\tau)\widetilde{B_i}(0)\right\rangle_B \tag{324}$$

$$= \Lambda_{ji}(\tau) \tag{325}$$

$$\mathrm{Tr}_B\left(\widetilde{B_j}(t)\rho_B^{\mathrm{Thermal}}\widetilde{B_i}(s)\right) = \mathrm{Tr}_B\left(\widetilde{B_i}(s)\widetilde{B_j}(t)\rho_B^{\mathrm{Thermal}}\right) \tag{326}$$

$$= \left\langle\widetilde{B_i}(s)\widetilde{B_j}(t)\right\rangle_B \tag{327}$$

$$= \left\langle\widetilde{B_i}(-\tau)\widetilde{B_j}(0)\right\rangle_B \tag{328}$$

$$= \Lambda_{ij}(-\tau) \tag{329}$$

$$\mathrm{Tr}_B\left(\widetilde{B_i}(s)\rho_B^{\mathrm{Thermal}}\widetilde{B_j}(t)\right) = \mathrm{Tr}_B\left(\widetilde{B_j}(t)\widetilde{B_i}(s)\rho_B^{\mathrm{Thermal}}\right) \tag{330}$$

$$= \left\langle\widetilde{B_j}(t)\widetilde{B_i}(s)\right\rangle_B \tag{331}$$

$$= \left\langle\widetilde{B_j}(\tau)\widetilde{B_i}(0)\right\rangle_B \tag{332}$$

$$= \Lambda_{ji}(\tau) \tag{333}$$

$$\mathrm{Tr}_B\left(\rho_B^{\mathrm{Thermal}}\widetilde{B_i}(s)\widetilde{B_j}(t)\right) = \mathrm{Tr}_B\left(\widetilde{B_i}(s)\widetilde{B_j}(t)\rho_B^{\mathrm{Thermal}}\right) \tag{334}$$

$$= \left\langle\widetilde{B_i}(s)\widetilde{B_j}(t)\right\rangle_B \tag{335}$$

$$= \left\langle\widetilde{B_i}(-\tau)\widetilde{B_j}(0)\right\rangle_B \tag{336}$$

$$= \Lambda_{ij}(-\tau) \tag{337}$$

The cyclic property of the trace was use widely in the development of equations (323) and (337). Replacing in (314)

$$\frac{\mathrm{d}\widetilde{\overline{\rho_S}}(t)}{\mathrm{d}t} = -\int_0^t \sum_{ij} \left(C_i(t) C_j(s) \left(\Lambda_{ij}(\tau) \, \widetilde{A}_i(t) \, \widetilde{A}_j(s) \widetilde{\overline{\rho_S}}(t) - \Lambda_{ji}(-\tau) \, \widetilde{A}_i(t) \widetilde{\overline{\rho_S}}(t) \widetilde{A}_j(s) \right) \right. \tag{338}$$

$$\left. + C_i(t) C_j(s) \left(\Lambda_{ji}(-\tau) \widetilde{\overline{\rho_S}}(t) \widetilde{A}_j(s) \, \widetilde{A}_i(t) - \Lambda_{ij}(\tau) \, \widetilde{A}_j(s) \widetilde{\overline{\rho_S}}(t) \widetilde{A}_i(t) \right) \right) \mathrm{d}s \tag{339}$$

$$= -\int_0^t \sum_{ij} \left(C_i(t) C_j(s) \left(\Lambda_{ij}(\tau) \left[\widetilde{A}_i(t), \widetilde{A}_j(s) \widetilde{\overline{\rho_S}}(t) \right] + \Lambda_{ji}(-\tau) \left[\widetilde{\overline{\rho_S}}(t) \widetilde{A}_j(s), \widetilde{A}_i(t) \right] \right) \right) \mathrm{d}s \tag{340}$$

We could identify the following commutators in the equation deduced:

$$\Lambda_{ij}(\tau) \, \widetilde{A}_i(t) \, \widetilde{A}_j(s) \widetilde{\overline{\rho_S}}(t) - \Lambda_{ij}(\tau) \, \widetilde{A}_j(s) \widetilde{\overline{\rho_S}}(t) \widetilde{A}_i(t) = \Lambda_{ij}(\tau) \left[\widetilde{A}_i(t), \widetilde{A}_j(s) \widetilde{\overline{\rho_S}}(t) \right] \tag{341}$$

$$\Lambda_{ji}(-\tau) \widetilde{\overline{\rho_S}}(t) \widetilde{A}_j(s) \, \widetilde{A}_i(t) - \Lambda_{ji}(-\tau) \, \widetilde{A}_i(t) \widetilde{\overline{\rho_S}}(t) \widetilde{A}_j(s) = \Lambda_{ji}(-\tau) \left[\widetilde{\overline{\rho_S}}(t) \widetilde{A}_j, \widetilde{A}_i(t) \right] \tag{342}$$

Returning to the interaction picture we have:

$$U(t) \, \widetilde{A}_i(t) \, \widetilde{A}_j(s) \widetilde{\overline{\rho_S}}(t) U^\dagger(t) = U(t) \, \widetilde{A}_i(t) \, U^\dagger(t) \, U(t) \, \widetilde{A}_j(s) \, U^\dagger(t) \, U(t) \widetilde{\overline{\rho_S}}(t) U^\dagger(t) \tag{343}$$

$$= \left(U(t) \, \widetilde{A}_i(t) \, U^\dagger(t) \right) \left(U(t) \, \widetilde{A}_j(s) \, U^\dagger(t) \right) \left(U(t) \widetilde{\overline{\rho_S}}(t) U^\dagger(t) \right) \tag{344}$$

$$= A_i \widetilde{A}_j(s, t) \, \overline{\rho_S}(t) \tag{345}$$

This procedure applying to the relevant commutators give us:

$$U(t) \left[\widetilde{A}_i(t), \widetilde{A}_j(s) \widetilde{\overline{\rho_S}}(t) \right] U^\dagger(t) = \left(U(t) \, \widetilde{A}_i(t) \, \widetilde{A}_j(s) \widetilde{\overline{\rho_S}}(t) U^\dagger(t) - U(t) \, \widetilde{A}_j(s) \widetilde{\overline{\rho_S}}(t) \widetilde{A}_i(t) \, U^\dagger(t) \right) \tag{346}$$

$$= A_i \widetilde{A}_j(s, t) \, \overline{\rho_S}(t) - \widetilde{A}_j(s, t) \, \overline{\rho_S}(t) A_i \tag{347}$$

$$= \left[A_i, \widetilde{A}_j(t - \tau, t) \, \overline{\rho_S}(t) \right] \tag{348}$$

Introducing this transformed commutators in the equation (340) allow us to obtain the master equation of the system

$$\frac{\mathrm{d}\overline{\rho_S}(t)}{\mathrm{d}t} = -\mathrm{i} \left[H_S(t), \overline{\rho_S}(t) \right] - \sum_{ij} \int_0^t \mathrm{d}\tau \left(C_i(t) C_j(t - \tau) \Lambda_{ij}(\tau) \left[A_i, \widetilde{A}_j(t - \tau, t) \, \overline{\rho_S}(t) \right] \right. \tag{349}$$

$$\left. + C_j(t) C_i(t - \tau) \Lambda_{ji}(-\tau) \left[\overline{\rho_S}(t) \widetilde{A}_j(t - \tau, t), A_i \right] \right) \tag{350}$$

where $i, j \in \{1, 2, 3, 4, 5.6\}$.

Here $\widetilde{A}_j(s, t) = U(t) U^\dagger(s) A_j U(s) U^\dagger(t)$ where $U(t)$ is given by (302). The equation obtained is a non-Markovian master equation which describes the QD exciton dynamics in the variational frame with a general time-dependent Hamiltonian, and valid at second order in $H_I(t)$. The environmental correlation functions are given by:

$$\Lambda_{ij}(\tau) = \mathrm{Tr}_B \left(\widetilde{B}_i(t) \, \widetilde{B}_j(s) \, \rho_B^{\mathrm{Thermal}} \right) \tag{351}$$

$$= \mathrm{Tr}_B \left(\widetilde{B}_i(\tau) \, \widetilde{B}_j(0) \, \rho_B^{\mathrm{Thermal}} \right) \tag{352}$$

Using the coherent-state representation of the bath density operator we find that the correlation functions are equal to:

$$\Lambda_{11}(\tau) = \mathrm{Tr}_B\left(\widetilde{B_1}(\tau)\widetilde{B_1}(0)\rho_B^{\mathrm{Thermal}}\right) \tag{353}$$

$$= \frac{B(\tau)B(0)}{2}\left(\mathrm{e}^{\phi(\tau)} + \mathrm{e}^{-\phi(\tau)} - 2\right) \tag{354}$$

$$\Lambda_{22}(\tau) = \mathrm{Tr}_B\left(\widetilde{B_2}(\tau)\widetilde{B_2}(0)\rho_B^{\mathrm{Thermal}}\right) \tag{355}$$

$$= \frac{B(\tau)B(0)}{2}\left(\mathrm{e}^{\phi(\tau)} + \mathrm{e}^{-\phi(\tau)}\right) \tag{356}$$

$$\Lambda_{33}(\tau) = \int_0^\infty \mathrm{d}\omega\, J(\omega)\left(1 - F(\omega)\right)^2 G_+(\tau) \tag{357}$$

$$\Lambda_{32}(\tau) = B(\tau)\int_0^\infty \mathrm{d}\omega\,\frac{J(\omega)}{\omega}F(\omega)\left(1 - F(\omega)\right)\mathrm{i}G_-(\tau) \tag{358}$$

$$\Lambda_{23}(\tau) = -B(0)\int_0^\infty \mathrm{d}\omega\,\frac{J(\omega)}{\omega}F(\omega,\tau)\left(1 - F(\omega,\tau)\right)\mathrm{i}G_-(\tau) \tag{359}$$

$$\Lambda_{12}(\tau) = \Lambda_{21}(\tau) = \Lambda_{13}(\tau) = \Lambda_{31}(\tau) = 0 \tag{360}$$

With the phonon propagator given by:

$$\phi(\tau) = \int_0^\infty \mathrm{d}\omega\,\frac{J(\omega)}{\omega^2}F(\omega)^2 G_+(\tau) \tag{361}$$

defined in terms of $G_\pm(\tau) = (n(\omega) + 1)\,\mathrm{e}^{-\mathrm{i}\tau\omega} \pm n(\omega)\,\mathrm{e}^{-\mathrm{i}\tau\omega}$ with $n(\omega) = \left(\mathrm{e}^{\beta\omega} - 1\right)^{-1}$ the occupation number. The matrix $\Lambda(\tau)$ called correlation matrix defined in terms of the equation (351) allows us to write all the correlations functions as:

$$\Lambda(\tau) = \begin{pmatrix} \Lambda_{11}(\tau) & 0 & 0 & 0 & -\Lambda_{11}(\tau) \\ 0 & \Lambda_{22}(\tau) & \Lambda_{23}(\tau) & \Lambda_{22}(\tau) & 0 \\ 0 & \Lambda_{32}(\tau) & \Lambda_{33}(\tau) & \Lambda_{32}(\tau) & 0 \\ 0 & \Lambda_{22}(\tau) & \Lambda_{23}(\tau) & \Lambda_{22}(\tau) & 0 \\ -\Lambda_{11}(\tau) & 0 & 0 & 0 & \Lambda_{11}(\tau) \end{pmatrix} \tag{362}$$

The eigenvalues of the Hamiltonian $\overline{H_S}$ are given by the solution of the following algebraic equation:

$$\lambda^2 - \mathrm{Tr}\left(\overline{H_S}\right)\lambda + \mathrm{Det}\left(\overline{H_S}\right) = 0 \tag{363}$$

The solutions of this equation written in terms of η and ξ as defined in the previous section are given by $\lambda_\pm = \frac{\xi \pm \eta}{2}$ and they satisfy $H_S\,|\pm\rangle = \lambda_\pm\,|\pm\rangle$. Using this notation is possible to write $H_S = \lambda_+\,|+\rangle\langle+| + \lambda_-\,|-\rangle\langle-|$.

The time-dependence of the system operators $\widetilde{A_i}(t)$ may be made explicit using the Fourier decomposition:

$$\widetilde{A_i}(\tau) = e^{\mathrm{i}\overline{H_S}\tau}A_i e^{-\mathrm{i}\overline{H_S}\tau} \tag{364}$$

$$= \sum_w e^{-\mathrm{i}w\tau}A_i(w) \tag{365}$$

Where the sum is defined on the set of all the differences between the eigenvalues of the system, in our case $w \in \{0, \pm\eta\}$.

In order to use the equation (365) to descompose the equation (302) we need to consider the time ordering operator $\mathcal{T}$, it's possible to write using the Dyson series or the expansion of the operator of the form $U(t) \equiv \mathcal{T}\exp\left(-\mathrm{i}\int_0^t \mathrm{d}v\overline{H_S}(v)\right)$ like:

$$U(t) \equiv \mathcal{T}\exp\left(-\mathrm{i}\int_0^t \mathrm{d}v \overline{H_S}(v)\right) \tag{366}$$

$$= \mathbb{I} + \sum_{n=1}^{\infty} (-\mathrm{i})^n \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 ... \int_0^{t_{n-1}} \mathrm{d}t_n H(t_1) H(t_2) ... H(t_n) \tag{367}$$

Here $0 < t_1 < t_2 < ... < t_{n-1} < t_n = t$ is a partition of the set $[0, t]$. We will use a perturbative solution to the exponential of a time-varying operator, this can be done if we write an effective hamiltonian $H_E(t)$ such that $\mathcal{T}\exp\left(-\mathrm{i}\int_0^t \mathrm{d}v \overline{H_S}(v)\right) \equiv \exp(-\mathrm{i}t H_E(t))$. The effective Hamiltonian is expanded in a series of terms of increasing order in time $H_E(t) = H_E^{(0)}(t) + H_E^{(1)}(t) + H_E^{(2)}(t) + ...$ so we can write:

$$U(t) = \exp\left(-\mathrm{i}t\left(H_E^{(0)}(t) + H_E^{(1)}(t) + H_E^{(2)}(t) + ...\right)\right) \tag{368}$$

The terms can be found expanding $\mathcal{T}\exp\left(-\mathrm{i}\int_0^t \mathrm{d}v \overline{H_S}(v)\right)$ and $U(t)$ then equating the terms of the same power. The lowest terms are:

$$H_E^{(0)}(t) = \frac{1}{t}\int_0^t \overline{H_S}(t')\,\mathrm{d}t' \tag{369}$$

$$H_E^{(1)}(t) = -\frac{\mathrm{i}}{2t}\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \left[\overline{H_S}(t'), \overline{H_S}(t'')\right] \tag{370}$$

$$H_E^{(2)}(t) = \frac{1}{6t}\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \int_0^{t''} \mathrm{d}t''' \left(\left[\left[\overline{H_S}(t'), \overline{H_S}(t'')\right], \overline{H_S}(t''')\right] + \left[\left[\overline{H_S}(t'''), \overline{H_S}(t'')\right], \overline{H_S}(t')\right]\right) \tag{371}$$

In this case the Fourier decomposition using the Magnus expansion is

$$\widetilde{A_i}(t) = e^{\mathrm{i}H_E(t)t} A_i(t) e^{-\mathrm{i}H_E(t)t} \tag{372}$$

$$= \sum_{w(t)} e^{-\mathrm{i}w(t)t} A_i(w(t)) \tag{373}$$

$w(t)$ belongs to the set of differences of eigenvalues that depends of the time. As we can see the eigenvectors are time dependent as well.

Extending the Fourier decomposition to the matrix $\widetilde{A_j}(t - \tau, t)$ using the Magnus expansion generates:

$$\widetilde{A_j}(t - \tau, t) = U(t - \tau) U^\dagger(t) A_j(t) U(t) U^\dagger(t - \tau) \tag{374}$$

$$= e^{-\mathrm{i}(t-\tau)H_E(t-\tau)} e^{\mathrm{i}H_E(t)t} A_j(t) e^{-\mathrm{i}H_E(t)t} e^{\mathrm{i}(t-\tau)H_E(t-\tau)} \tag{375}$$

$$= e^{-\mathrm{i}(t-\tau)H_E(t-\tau)} \sum_{w(t)} e^{-\mathrm{i}w(t)t} A_j(w(t)) e^{\mathrm{i}(t-\tau)H_E(t-\tau)} \tag{376}$$

$$= \sum_{w(t), w'(t-\tau)} e^{-\mathrm{i}w(t)t} e^{\mathrm{i}w'(t-\tau)} A'_j(w(t), w'(t-\tau)) \tag{377}$$

where $w'(t - \tau)$ and $w(t)$ belongs to the set of the differences of the eigenvalues of the Hamiltonian $H_S(t - \tau)$ and $H_S(t)$ respectively.

In order to show the explicit form of the matrices present in the RHS of the equation (365) for a general 2×2 matrix in a given time let's write the matrix A_i in the base $\mathrm{V} = \{|+\rangle, |-\rangle\}$ in the following way:

$$A_i = \sum_{\alpha, \beta \in \mathrm{V}} \langle\alpha| A_i |\beta\rangle |\alpha\rangle \langle\beta| \tag{378}$$

Given that $[|+\rangle\langle+|,|-\rangle\langle-|] = 0$, then using the Zassenhaus formula we obtain:

$$e^{i\overline{H_S}\tau} = e^{i(\lambda_+|+\rangle\langle+|+\lambda_-|-\rangle\langle-|)\tau} \tag{379}$$

$$= e^{i\lambda_+|+\rangle\langle+|\tau}e^{i\lambda_-|-\rangle\langle-|\tau} \tag{380}$$

$$= \left(|-\rangle\langle-| + e^{i\lambda_+\tau}|+\rangle\langle+|\right)\left(|+\rangle\langle+| + e^{i\lambda_-\tau}|-\rangle\langle-|\right) \tag{381}$$

$$= e^{i\lambda_+\tau}|+\rangle\langle+| + e^{i\lambda_-\tau}|-\rangle\langle-| \tag{382}$$

Calculating the transformation (365) directly using the previous relationship we find that:

$$\widetilde{A_i}(\tau) = \left(e^{i\lambda_+\tau}|+\rangle\langle+| + e^{i\lambda_-\tau}|-\rangle\langle-|\right)\left(\sum_{\alpha,\beta\in V}\langle\alpha|A_i|\beta\rangle|\alpha\rangle\langle\beta|\right)\left(e^{-i\lambda_+\tau}|+\rangle\langle+| + e^{-i\lambda_-\tau}|-\rangle\langle-|\right) \tag{383}$$

$$= \langle+|A_i|+\rangle|+\rangle\langle+| + e^{i\eta\tau}\langle+|A_i|-\rangle|+\rangle\langle-| + e^{-i\eta\tau}\langle-|A_i|+\rangle|-\rangle\langle+| + \langle-|A_i|-\rangle|-\rangle\langle-| \tag{384}$$

Here $\eta = \lambda_+ - \lambda-$. Comparing the RHS of the equations (365) and the explicit expression for $\widetilde{A_i}(\tau)$ and we obtain the form of the expansion matrices of the Fourier decomposition for a general 2×2 matrix:

$$A_i(0) = \langle+|A_i|+\rangle|+\rangle\langle+| + \langle-|A_i|-\rangle|-\rangle\langle-| \tag{385}$$

$$A_i(w) = \langle+|A_i|-\rangle|+\rangle\langle-| \tag{386}$$

$$A_i(-w) = \langle-|A_i|+\rangle|-\rangle\langle+| \tag{387}$$

For a decomposition of the interaction Hamiltonian in terms of Hermitian operators, i.e. $\widetilde{A_i}(\tau) = \widetilde{A_i}^\dagger(\tau)$ and $\widetilde{B_i}(\tau) = \widetilde{B_i}^\dagger(\tau)$ we can use the equation (365) to write the master equation in the following neater form:

$$\frac{d\overline{\rho}_S}{dt} = -i[H_S(t),\overline{\rho}_S(t)] - \frac{1}{2}\sum_{ij}\sum_{w,w'}\gamma_{ij}(w,w',t)\left[A_i,A_j(w,w')\overline{\rho}_S(t) - \overline{\rho}_S(t)A_j^\dagger(w,w')\right] - \sum_{ij}\sum_w S_{ij}(w,w',t)\left[A_i,A_j(w,w')\overline{\rho}_S(t) + \overline{\rho}_S(t)A_j^\dagger(w,w')\right] \tag{388}$$

where $A_j^\dagger(w) = A(-w)$ as expected from the equations (386) and (387). As we can see the equation shown contains the rates and energy shifts $\gamma_{ij}(w,w',t) = 2\Re(K_{ij}(w,w',t))$ and $S_{ij}(w,w',t) = \Im(K_{ij}(w,w',t))$, respectively, defined in terms of the response functions

$$K_{ij}(w,w',t) = \int_0^t C_i(t)C_j(t-\tau)\Lambda_{ij}(\tau)e^{iw\tau}e^{-it(w-w')}d\tau \tag{389}$$

If we extend the upper limit of integration to ∞ in the equation (389) then the system will be independent of any preparation at $t = 0$, so the evolution of the system will depend only on its present state as expected in the Markovian approximation.

V. LIMIT CASES

In order to show the plausibility of the master equation (388) for a time-dependent Hamiltonian we will show that this equation reproduces the following cases under certain limits conditions that will be pointed in each subsection.

A. Time-independent variational quantum master equation

At first let's show that the master equation (388) reproduces the results of the reference [1], for the latter case we have that $i,j \in \{1,2,3\}$ and $\omega \in (0,\pm\eta)$. The Hamiltonian of the system considered in this reference written in the same basis than the Hamiltonian (1) is given by:

$$H = \left(\delta + \sum_j g_k \left(b_k^\dagger + b_k\right)\right) |1\rangle\langle 1| + \frac{\Omega}{2}\sigma_x + \sum_k \omega_k b_k^\dagger b_k \tag{390}$$

After performing the transformation (24) on the Hamiltonian (390) it's possible to split that result in the following set of Hamiltonians:

$$\overline{H_S} = (\delta + R) |1\rangle\langle 1| + \frac{\Omega_r}{2}\sigma_x \tag{391}$$

$$\overline{H_I} = B_z |1\rangle\langle 1| + \frac{\Omega}{2}\left(B_x\sigma_x + B_y\sigma_y\right) \tag{392}$$

$$H_B = \sum_k \omega_k b_k^\dagger b_k \tag{393}$$

The Hamiltonian (391) differs from the transformed Hamiltonian H_S of the reference written like $H_S = \frac{R}{2}\mathbb{I} + \frac{\epsilon}{2}\sigma_z + \frac{\Omega_r}{2}\sigma_x$ by a term proportional to the identity, this can be seen in the following way taking $\epsilon = \delta + R$

$$(\delta + R) |1\rangle\langle 1| - \frac{\delta}{2}\mathbb{I} = \left(\frac{\delta}{2} + R\right) |1\rangle\langle 1| - \frac{\delta}{2}|0\rangle\langle 0| \tag{394}$$

$$= \frac{R}{2}\mathbb{I} + \frac{\delta + R}{2}\sigma_z \tag{395}$$

$$= \frac{R}{2}\mathbb{I} + \frac{\epsilon}{2}\sigma_z \tag{396}$$

In this Hamiltonian we can write $A_i = \sigma_x$, $A_2 = \sigma_y$ and $A_3 = \frac{I+\sigma_z}{2}$. In order to find the decomposition matrices of the Fourier decomposition let's obtain the eigenvalues and eigenvectors of the matrix $\overline{H_S}$.

$$\lambda_+ = \frac{\epsilon + \eta}{2} \tag{397}$$

$$\lambda_- = \frac{\epsilon - \eta}{2} \tag{398}$$

$$|+\rangle = \frac{1}{\sqrt{(\epsilon + \eta)^2 + \Omega_r^2}} \begin{pmatrix} \epsilon + \eta \\ \Omega_r \end{pmatrix} \tag{399}$$

$$|-\rangle = \frac{1}{\sqrt{(\epsilon + \eta)^2 + \Omega_r^2}} \begin{pmatrix} -\Omega_r \\ \epsilon + \eta \end{pmatrix} \tag{400}$$

Using this basis we can find the decomposition matrices using the equations (386)-(387) and the fact that $|+\rangle = \cos(\theta)|1\rangle + \sin(\theta)|0\rangle$ and $|-\rangle = -\sin(\theta)|1\rangle + \cos(\theta)|0\rangle$ with$\sin(\theta) = \frac{\Omega_r}{\sqrt{(\epsilon+\eta)^2+\Omega_r^2}}$ and $\cos(\theta) = \frac{\epsilon+\eta}{\sqrt{(\epsilon+\eta)^2+\Omega_r^2}}$:

$$\langle +|\,\sigma_x\,|+\rangle = \begin{pmatrix} \cos\left(\theta\right) & \sin\left(\theta\right) \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos\left(\theta\right) \\ \sin\left(\theta\right) \end{pmatrix} \tag{401}$$

$$= 2\sin\left(\theta\right)\cos\left(\theta\right) \tag{402}$$

$$= \sin\left(2\theta\right) \tag{403}$$

$$\langle -|\,\sigma_x\,|-\rangle = \begin{pmatrix} -\sin\left(\theta\right) & \cos\left(\theta\right) \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} -\sin\left(\theta\right) \\ \cos\left(\theta\right) \end{pmatrix} \tag{404}$$

$$= -2\sin\left(\theta\right)\cos\left(\theta\right) \tag{405}$$

$$= -\sin\left(2\theta\right) \tag{406}$$

$$\langle -|\,\sigma_x\,|+\rangle = \begin{pmatrix} -\sin\left(\theta\right) & \cos\left(\theta\right) \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos\left(\theta\right) \\ \sin\left(\theta\right) \end{pmatrix} \tag{407}$$

$$= \cos^2\left(\theta\right) - \sin^2\left(\theta\right) \tag{408}$$

$$= \cos\left(2\theta\right) \tag{409}$$

$$\langle +|\,\sigma_y\,|+\rangle = \begin{pmatrix} \cos\left(\theta\right) & \sin\left(\theta\right) \end{pmatrix} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \begin{pmatrix} \cos\left(\theta\right) \\ \sin\left(\theta\right) \end{pmatrix} \tag{410}$$

$$= \mathrm{i}\sin\left(\theta\right)\cos\left(\theta\right) - \mathrm{i}\sin\left(\theta\right)\cos\left(\theta\right) \tag{411}$$

$$= 0 \tag{412}$$

$$\langle -|\,\sigma_y\,|-\rangle = \begin{pmatrix} -\sin\left(\theta\right) & \cos\left(\theta\right) \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} -\sin\left(\theta\right) \\ \cos\left(\theta\right) \end{pmatrix} \tag{413}$$

$$= -\mathrm{i}\sin\left(\theta\right)\cos\left(\theta\right) + \mathrm{i}\sin\left(\theta\right)\cos\left(\theta\right) \tag{414}$$

$$= 0 \tag{415}$$

$$\langle -|\,\sigma_y\,|+\rangle = \begin{pmatrix} -\sin\left(\theta\right) & \cos\left(\theta\right) \end{pmatrix} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \begin{pmatrix} \cos\left(\theta\right) \\ \sin\left(\theta\right) \end{pmatrix} \tag{416}$$

$$= \mathrm{i}\cos^2\left(\theta\right) + \mathrm{i}\sin^2\left(\theta\right) \tag{417}$$

$$= \mathrm{i} \tag{418}$$

$$\langle +|\,\frac{1+\sigma_z}{2}\,|+\rangle = \begin{pmatrix} \cos\left(\theta\right) & \sin\left(\theta\right) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cos\left(\theta\right) \\ \sin\left(\theta\right) \end{pmatrix} \tag{419}$$

$$= \cos\left(\theta\right)\cos\left(\theta\right) \tag{420}$$

$$= \cos^2\left(\theta\right) \tag{421}$$

$$\langle -|\,\frac{1+\sigma_z}{2}\,|-\rangle = \begin{pmatrix} -\sin\left(\theta\right) & \cos\left(\theta\right) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} -\sin\left(\theta\right) \\ \cos\left(\theta\right) \end{pmatrix} \tag{422}$$

$$= \sin\left(\theta\right)\sin\left(\theta\right) \tag{423}$$

$$= \sin^2\left(\theta\right) \tag{424}$$

$$\langle -|\,\frac{1+\sigma_z}{2}\,|+\rangle = \begin{pmatrix} -\sin\left(\theta\right) & \cos\left(\theta\right) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \cos\left(\theta\right) \\ \sin\left(\theta\right) \end{pmatrix} \tag{425}$$

$$= -\sin\left(\theta\right)\cos\left(\theta\right) \tag{426}$$

$$= -\sin\left(\theta\right)\cos\left(\theta\right) \tag{427}$$

Composing the parts shown give us the Fourier decomposition matrices for this case:

$$A_1\left(0\right) = \sin\left(2\theta\right)\left(|+\rangle\langle +| - |-\rangle\langle -|\right) \tag{428}$$

$$A_1\left(\eta\right) = \cos\left(2\theta\right)|-\rangle\langle +| \tag{429}$$

$$A_2\left(0\right) = 0 \tag{430}$$

$$A_2\left(\eta\right) = \mathrm{i}\,|-\rangle\langle +| \tag{431}$$

$$A_3\left(0\right) = \cos^2\left(\theta\right)|+\rangle\langle +| + \sin^2\left(\theta\right)|-\rangle\langle -| \tag{432}$$

$$A_3\left(\eta\right) = -\sin\left(\theta\right)\cos\left(\theta\right)|-\rangle\langle +| \tag{433}$$

Now to make comparisons between the model obtained and the model of the system under discussion we will define that the correlation functions of the reference [1] denoted by $\Lambda'_{ij}(\tau)$ relate with the correlation functions defined in the equation (352) in the following way:

$$\Lambda'_{ij}(\tau) = C_i(t)\, C_j(t-\tau)\, \Lambda_{ij}(\tau) \tag{434}$$

Using the notation of the master equation (388), we can say that $C_1(t) = \frac{\Omega}{2} = C_2(t)$ and $C_3(t) = 1$, being Ω a constant. Furthermore given that $\overline{H_S}$ is time-independent then $B(t) = B$. Taking the equations (353)-(360) we find that the correlation functions of the reference [1] written in terms of the RHS of the equation (352) are equal to:

$$\Lambda'_{11}(\tau) = \left(\frac{\Omega}{2}\right)^2 \mathrm{Tr}_B\left(\widetilde{B_1}(\tau)\,\widetilde{B_1}(0)\,\rho_B\right) \tag{435}$$

$$= \frac{\Omega_r^2}{8}\left(e^{\phi(\tau)} + e^{-\phi(\tau)} - 2\right) \tag{436}$$

$$\Lambda'_{22}(\tau) = \left(\frac{\Omega}{2}\right)^2 \mathrm{Tr}_B\left(\widetilde{B_2}(\tau)\,\widetilde{B_2}(0)\,\rho_B\right) \tag{437}$$

$$= \frac{\Omega_r^2}{8}\left(e^{\phi(\tau)} + e^{-\phi(\tau)}\right) \tag{438}$$

$$\Lambda'_{33}(\tau) = \int_0^\infty d\omega\, J(\omega)\,(1 - F(\omega))^2\, G_+(\tau) \tag{439}$$

$$\Lambda'_{32}(\tau) = \frac{\Omega_r}{2}\int_0^\infty d\omega\, \frac{J(\omega)}{\omega}\, F(\omega)\,(1 - F(\omega))\, iG_-(\tau) \tag{440}$$

$$\Lambda'_{32}(\tau) = -\Lambda'_{23}(\tau) \tag{441}$$

$$\Lambda'_{12}(\tau) = \Lambda'_{21}(\tau) = \Lambda'_{13}(\tau) = \Lambda'_{31}(\tau) = 0 \tag{442}$$

Finally taking the Hamiltonian (390) and given that to reproduce this Hamiltonian we need to impose in (5) that $V_{10}(t) = \frac{\Omega}{2}$, $\varepsilon_0(t) = 0$ and $\varepsilon_1(t) = \delta$, then we obtain that $\mathrm{Det}\left(\overline{H_S}\right) = -\frac{\Omega_r^2}{4}$, $\mathrm{Tr}\left(\overline{H_S}\right) = \epsilon$. Now $\eta = \sqrt{\epsilon^2 + \Omega_r^2}$ and using the equation (286) we have that:

$$f_k = \frac{g_k\left(1 - \frac{\epsilon \tanh\left(\frac{\beta\eta}{2}\right)}{\eta}\right)}{1 - \frac{\tanh\left(\frac{\beta\eta}{2}\right)}{\eta}\left(\epsilon - \frac{\Omega_r^2 \coth\left(\frac{\beta\omega_k}{2}\right)}{2\omega_k}\right)} \tag{443}$$

$$= \frac{g_k\left(1 - \frac{\epsilon \tanh\left(\frac{\beta\eta}{2}\right)}{\eta}\right)}{1 - \frac{\epsilon \tanh\left(\frac{\beta\eta}{2}\right)}{\eta}\left(1 - \frac{\Omega_r^2 \coth\left(\frac{\beta\omega_k}{2}\right)}{2\epsilon\omega_k}\right)} \tag{444}$$

This shows that the expression obtained reproduces the variational parameters of the time-independent model of the reference. In general we can see that the time-independent model studied can be reproduced using the master equation (350) under a time-independent approach providing similar results.

Given that the Hamiltonian of this system is time-independent, then $U(t)\,U^\dagger(t-\tau) = U(\tau)$. From the equation (388) and using the fact that

$$\widetilde{A_j}(t-\tau, t) = U(\tau)\, A_j\, U(-\tau) \tag{445}$$

$$= \sum_w e^{iw\tau}\, A_i(-w) \tag{446}$$

$$= \sum_w e^{-iw\tau}\, A_i(w) \tag{447}$$

because the matrices $U(t)$ and $U(t-\tau)$ commute from the fact that $H_S(t)$ and $H_S(t-\tau)$ commute as well for time independent Hamiltonians. The master equation is equal to:

$$\frac{\mathrm{d}\overline{\rho_S}(t)}{\mathrm{d}t} = -\mathrm{i}\left[H_S(t), \overline{\rho_S}(t)\right] - \frac{1}{2}\sum_{ij}\sum_{w}\gamma_{ij}(w,t)\left[A_i, A_j(w)\overline{\rho}_S(t) - \overline{\rho}_S(t)A_j^\dagger(w)\right] \tag{448}$$

$$- \sum_{ij}\sum_{w}S_{ij}(w,t)\left[A_i, A_j(w)\overline{\rho}_S(t) + \overline{\rho}_S(t)A_j^\dagger(w)\right] \tag{449}$$

where $A_j^\dagger(w) = A(-w)$, as we can see the equation (449) contains the rates and energy shifts $\gamma_{ij}(w,t) = 2\Re(K_{ij}(w,t))$ and $S_{ij}(w,t) = \Im(K_{ij}(w,t))$, respectively, defined in terms of the response functions

$$K_{ij}(w,t) = \int_0^t \Lambda'_{ij}(\tau)e^{\mathrm{i}w\tau}\mathrm{d}\tau \tag{450}$$

B. Time-dependent polaron quantum master equation

Following the reference [1], when $\Omega_k \ll \omega_k$ then $f_k \approx g_k$ so we recover the full polaron transformation. It means from the equation (118) that $B_z = 0$. The Hamiltonian studied is given by:

$$H = \left(\delta + \sum_{\mathbf{k}}\left(g_{\mathbf{k}}b_{\mathbf{k}}^\dagger + g_{\mathbf{k}}^* b_{\mathbf{k}}\right)\right)|1\rangle\langle1| + \frac{\Omega(t)}{2}\sigma_x + \sum_k \omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \tag{451}$$

If $v_{\mathbf{k}} \approx g_{\mathbf{k}}$ then $B(\tau) = B$, so B is independent of the time. In order to reproduce the Hamiltonian of the equation (451) using the Hamiltonian of the equation (1) we can say that $\delta = \varepsilon_1(t)$, $\varepsilon_0(t) = 0$, $V_{10}(t) = \frac{\Omega(t)}{2}$. Now given that $v_{\mathbf{k}} \approx g_{\mathbf{k}}$ then, in this case and using the equation (225) and (236) we obtain the following transformed Hamiltonians:

$$\overline{H_S} = (\delta + R_1)|1\rangle\langle1| + \frac{B\sigma_x}{2}\Omega(t) \tag{452}$$

$$\overline{H_I} = \frac{\Omega(t)}{2}(B_x\sigma_x + B_y\sigma_y) \tag{453}$$

In this case $R_1 = \sum_{\mathbf{k}}\left(\omega_{\mathbf{k}}\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} - 2\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}g_{\mathbf{k}}\right)$ from (27) and given that $v_{\mathbf{k}} \approx g_{\mathbf{k}}$ and $\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} = g_{\mathbf{k}}/\omega_{\mathbf{k}}$ then $R_1 = \sum_{\mathbf{k}}\left(-\omega_{\mathbf{k}}^{-1}|g_{\mathbf{k}}|^2\right) = \sum_{\mathbf{k}}\left(-\omega_{\mathbf{k}}|\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}|^2\right)$ as expected, take $\delta + R_1 = \delta'$. If $F(\omega_{\mathbf{k}}) = 1$ and using the equations (353)-(360) we can deduce that the only terms that survive are $\Lambda_{11}(\tau)$ and $\Lambda_{22}(\tau)$. The phonon propagator for this case is:

$$\phi(\tau) = \int_0^\infty \frac{J(\omega)}{\omega^2}G_+(\tau)\mathrm{d}\omega \tag{454}$$

Writing $G_+(\tau) = \coth\left(\frac{\beta\omega}{2}\right)\cos(\omega\tau) - i\sin(\omega\tau)$ so (454) can be written as:

$$\phi(\tau) = \int_0^\infty \frac{J(\omega)}{\omega^2}\left(\coth\left(\frac{\beta\omega}{2}\right)\cos(\omega\tau) - i\sin(\omega\tau)\right)\mathrm{d}\omega \tag{455}$$

Writing the interaction Hamiltonian (453) in the similar way to the equation (236) allow us to to write $A_1 = \sigma_x$, $A_2 = \sigma_y$, $B_1(t) = B_x$, $B_2(t) = B_y$ and $C_1(t) = \frac{\Omega(t)}{2} = C_2(t)$. Now taking the equation (225) with $\delta'|1\rangle\langle1| = \frac{\delta'}{2}\sigma_z + \frac{\delta'}{2}\mathbb{I}$ help us to reproduce the hamiltonian of the reference [2]. Then $\overline{H_S}$ is equal to:

$$\overline{H_S} = \frac{\delta'}{2}\sigma_z + \frac{B\sigma_x}{2}\Omega(t) \tag{456}$$

As we can see the function B is a time-independent function because we consider that $g_\mathbf{k}$ doesn't depend of the time. In this case the relevant correlation functions are given by:

$$\Lambda_{11}(\tau) = \text{Tr}_B\left(\widetilde{B_1}(\tau)\,\widetilde{B_1}(0)\,\rho_B\right) \tag{457}$$

$$= \frac{B^2}{2}\left(e^{\phi(\tau)} + e^{-\phi(\tau)} - 2\right) \tag{458}$$

$$\Lambda_{22}(\tau) = \text{Tr}_B\left(\widetilde{B_2}(\tau)\,\widetilde{B_2}(0)\,\rho_B\right) \tag{459}$$

$$= \frac{B^2}{2}\left(e^{\phi(\tau)} + e^{-\phi(\tau)}\right) \tag{460}$$

These functions match with the equations $\Lambda_x(\tau)$ and $\Lambda_y(\tau)$ of the reference [2] and $\Lambda_i(\tau) = \Lambda_i(-\tau)$ for $i \in \{x, y\}$ respectively. The master equation for this section based on the equation (350) is:

$$\frac{d\overline{\rho_S}(t)}{dt} = -i\left[\frac{\delta'}{2}\sigma_z + \frac{\Omega_r(t)\sigma_x}{2}, \rho_S(t)\right] - \sum_{i=1}^{2}\int_0^t d\tau\left(C_i(t)\,C_i(t-\tau)\,\Lambda_{ii}(\tau)\left[A_i, \widetilde{A_i}(t-\tau,t)\,\rho_S(t)\right]\right. \tag{461}$$

$$\left. + C_i(t)\,C_i(t-\tau)\,\Lambda_{ii}(-\tau)\left[\rho_S(t)\,\widetilde{A_i}(t-\tau,t), A_i\right]\right) \tag{462}$$

Replacing $C_i(t) = \frac{\Omega(t)}{2}$ and $\widetilde{A_i}(t-\tau,t) = \widetilde{\sigma_i}(t-\tau,t)$, also using the equations (457) and (460) on the equation (462) we obtain that:

$$\frac{d\overline{\rho_S}(t)}{dt} = -\frac{i}{2}\left[\delta'\sigma_z + \Omega_r(t)\sigma_x, \rho_S(t)\right] - \frac{\Omega(t)}{4}\int_0^t d\tau\,\Omega(t-\tau)\left(\left[\sigma_x, \widetilde{\sigma_x}(t-\tau,t)\,\rho_S(t)\right]\Lambda_x(\tau)\right. \tag{463}$$

$$\left. + \left[\sigma_y, \widetilde{\sigma_y}(t-\tau,t)\,\rho_S(t)\right]\Lambda_y(\tau) + \left[\rho_S(t)\,\widetilde{\sigma_x}(t-\tau,t), \sigma_x\right]\Lambda_x(\tau) + \left[\rho_S(t)\,\widetilde{\sigma_y}(t-\tau,t), \sigma_y\right]\Lambda_y(\tau)\right) \tag{464}$$

As we can see $\left[A_j, \widetilde{A_i}(t-\tau,t)\,\rho_S(t)\right]^\dagger = \left[\rho_S(t)\,\widetilde{A_i}(t-\tau,t), A_j\right]$, $\Lambda_x(\tau) = \Lambda_x(-\tau)$ and $\Lambda_y(\tau) = \Lambda_y(-\tau)$, so the result obtained is the same master equation (21) of the reference [2] extended in the hermitian conjugate.

<div align="center">

C. Time-Dependent Weak-Coupling Limit

</div>

In order to prove that the master equation deduced reproduces the equation $(S17)$ of the reference [3] we will impose that $F(\omega) = 0$, so there is no transformation in this case. As we can see from the definition (352) the only term that survives is $\Lambda_{33}(\tau)$. Taking $\bar{h} = 1$ the Hamiltonian of the reference can be written in the form:

$$H = \Delta|1\rangle\langle 1| + \frac{\Omega(t)}{2}\left(|1\rangle\langle 0| + |0\rangle\langle 1|\right) + \sum_\mathbf{k}\omega_\mathbf{k}b_\mathbf{k}^\dagger b_\mathbf{k} + |1\rangle\langle 1|\sum_\mathbf{k}\left(g_\mathbf{k}b_\mathbf{k}^\dagger + g_\mathbf{k}^* b_\mathbf{k}\right) \tag{465}$$

Using the equation (388), from the fact that the Hamiltonian is time-independent in the evolution time allow us to write:

$$\frac{d\rho_S}{dt} = -i\left[H_S(t), \rho_S(t)), \rho_S(t)\right] - \frac{1}{2}\sum_w\gamma_{33}(w,t)\left[A_3, A_3(w)\rho_S(t) - \rho_S(t)A_3^\dagger(w)\right] \tag{466}$$

$$- \sum_w S_{33}(w,t)\left[A_3, A_3(w)\rho_S(t) + \rho_S(t)A_3^\dagger(w)\right]\bigg) \tag{467}$$

The correlation functions are relevant if $F(\omega) = 0$ for the weak-coupling approximation are:

$$\Lambda_{33}(\tau) = \int_0^\infty \mathrm{d}\omega J(\omega) G_+(\tau) \tag{468}$$

$$\Lambda_{33}(-\tau) = \int_0^\infty \mathrm{d}\omega J(\omega) G_+(-\tau) \tag{469}$$

In our case $A_3 = \frac{\mathbb{I}+\sigma_z}{2}$, the equation (467) can be transformed in

$$\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = -\mathrm{i}[H_S(t), \rho_S(t)] - \sum_w \left(K_{33}(w,t)[A_3, A_3(w)\rho_S(t)] + K_{33}^*(w,t)[\rho_S(t)A_3(w), A_3] \right) \tag{470}$$

As the paper suggest we will consider that the quantum system is in resonance, so $\Delta = 0$ and furthemore, the relaxation time of the bath is less than the evolution time to be considered, so the frequency of the Rabi frequency of the laser can be taken as constant and equal to $\widetilde{\Omega}$ To find the matrices $A_3(w)$, we have to remember that $H_S = \frac{\Omega(t)}{2}(|1\rangle\langle 0| + |0\rangle\langle 1|)$, this Hamiltonian have the following eigenvalues and eigenvectors:

$$\lambda_+ = \frac{\widetilde{\Omega}}{2} \tag{471}$$

$$|+\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |0\rangle) \tag{472}$$

$$\lambda_- = -\frac{\widetilde{\Omega}}{2} \tag{473}$$

$$|-\rangle = \frac{1}{\sqrt{2}}(-|1\rangle + |0\rangle) \tag{474}$$

The elements of the decomposition matrices are:

$$\langle +|\frac{1+\sigma_z}{2}|+\rangle = \frac{1}{2}\begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{475}$$

$$= \frac{1}{2} \tag{476}$$

$$\langle -|\frac{1+\sigma_z}{2}|-\rangle = \frac{1}{2}\begin{pmatrix} -1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} -1 \\ 1 \end{pmatrix} \tag{477}$$

$$= \frac{1}{2} \tag{478}$$

$$\langle -|\frac{1+\sigma_z}{2}|+\rangle = \frac{1}{2}\begin{pmatrix} -1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{479}$$

$$= -\frac{1}{2} \tag{480}$$

The decomposition matrices are

$$A_3(0) = \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -| \tag{481}$$

$$= \frac{\mathbb{I}}{2} \tag{482}$$

$$A_3(\eta) = -\frac{1}{2}|-\rangle\langle +| \tag{483}$$

$$= \frac{1}{4}(\sigma_z + \mathrm{i}\sigma_y) \tag{484}$$

$$A_3(-\eta) = -\frac{1}{2}|+\rangle\langle -| \tag{485}$$

$$= \frac{1}{4}(\sigma_z - \mathrm{i}\sigma_y) \tag{486}$$

Neglecting the term proportional to the identity in the Hamiltonian we obtain that:

$$\frac{d\rho_S(t)}{dt} = -i\frac{\widetilde{\Omega}}{2}\left[\sigma_x, \rho_S\left(t\right)\right] - K_{33}\left(\widetilde{\Omega}, t\right)\left[\frac{\sigma_z}{2}, \frac{1}{4}\left(\sigma_z + i\sigma_y\right)\rho_S\left(t\right)\right] - K_{33}\left(-\widetilde{\Omega}, t\right)\left[\frac{\sigma_z}{2}, \frac{1}{4}\left(\sigma_z - i\sigma_y\right)\rho_S\left(t\right)\right] \tag{487}$$

$$- K_{33}^*\left(\widetilde{\Omega}, t\right)\left[\rho_S\left(t\right)\frac{1}{4}\left(\sigma_z + i\sigma_y\right), \frac{\sigma_z}{2}\right] - K_{33}^*\left(-\widetilde{\Omega}, t\right)\left[\rho_S\left(t\right)\frac{1}{4}\left(\sigma_z - i\sigma_y\right), \frac{\sigma_z}{2}\right] \tag{488}$$

Calculating the response functions extending the upper limit of τ to ∞, we obtain:

$$K_{33}\left(\widetilde{\Omega}\right) = \int_0^\infty \int_0^\infty J\left(\omega\right)G_+\left(\tau\right)e^{i\widetilde{\Omega}\tau}d\tau d\omega \tag{489}$$

$$= \int_0^\infty \int_0^\infty J\left(\omega\right)e^{i\widetilde{\Omega}\tau}\left(\left(n\left(\omega\right)+1\right)e^{-i\tau\omega}+n\left(\omega\right)e^{i\tau\omega}\right)d\tau d\omega \tag{490}$$

$$= \int_0^\infty \int_0^\infty J\left(\omega\right)e^{i\widetilde{\Omega}\tau}\left(n\left(\omega\right)+1\right)e^{-i\tau\omega}d\tau d\omega \tag{491}$$

$$= \int_0^\infty \int_0^\infty J\left(\omega\right)\left(n\left(\omega\right)+1\right)e^{i\widetilde{\Omega}\tau-i\tau\omega}d\tau d\omega \tag{492}$$

$$= \int_0^\infty J\left(\omega\right)\left(n\left(\omega\right)+1\right)\pi\delta\left(\widetilde{\Omega}-\omega\right)d\omega \tag{493}$$

$$= \pi J\left(\widetilde{\Omega}\right)\left(n\left(\widetilde{\Omega}\right)+1\right) \tag{494}$$

$$K_{33}\left(-\widetilde{\Omega}\right) = \int_0^\infty \int_0^\infty J\left(\omega\right)G_+\left(\tau\right)e^{-i\widetilde{\Omega}\tau}d\tau d\omega \tag{495}$$

$$= \int_0^\infty \int_0^\infty J\left(\omega\right)e^{-i\widetilde{\Omega}\tau}\left(\left(n\left(\omega\right)+1\right)e^{-i\tau\omega}+n\left(\omega\right)e^{i\tau\omega}\right)d\tau d\omega \tag{496}$$

$$= \int_0^\infty \int_0^\infty J\left(\omega\right)e^{-i\widetilde{\Omega}\tau}n\left(\omega\right)e^{i\tau\omega}d\tau d\omega \tag{497}$$

$$= \int_0^\infty \int_0^\infty J\left(\omega\right)n\left(\omega\right)e^{-i\widetilde{\Omega}\tau+i\tau\omega}d\tau d\omega \tag{498}$$

$$= \int_0^\infty J\left(\omega\right)n\left(\omega\right)\pi\delta\left(-\widetilde{\Omega}+\omega\right)d\omega \tag{499}$$

$$= \pi J\left(\widetilde{\Omega}\right)n\left(\widetilde{\Omega}\right) \tag{500}$$

Here we have used $\int_0^\infty ds\, e^{\pm i\varepsilon s} = \pi\delta\left(\varepsilon\right)\pm i\frac{V.P.}{\varepsilon}$, where V.P. denotes the Cauchy's principal value. Theses principal values are ignored because they lead to small renormalizations of the Hamiltonian. Furthermore we don't take account of value associated to the matrix $A_3\left(0\right)$ because the spectral density $J\left(\omega\right)$ is equal to zero when $\omega = 0$. Replacing in the equation (487) lead us to obtain:

$$\frac{d\rho_S(t)}{dt} = -i\frac{\widetilde{\Omega}}{2}\left[\sigma_x, \rho_S\left(t\right)\right] - \frac{\pi}{8}J\left(\widetilde{\Omega}\right)\left(\left(n\left(\widetilde{\Omega}\right)+1\right)\left[\sigma_z, \left(\sigma_z + i\sigma_y\right)\rho_S\left(t\right)\right] + n\left(\widetilde{\Omega}\right)\left[\sigma_z, \left(\sigma_z - i\sigma_y\right)\rho_S\left(t\right)\right]\right) \tag{501}$$

$$- \frac{\pi}{8}J\left(\widetilde{\Omega}\right)\left(\left(n\left(\widetilde{\Omega}\right)+1\right)\left[\rho_S\left(t\right)\left(\sigma_z + i\sigma_y\right), \sigma_z\right] + n\left(\widetilde{\Omega}\right)\left[\rho_S\left(t\right)\left(\sigma_z - i\sigma_y\right), \sigma_z\right]\right) \tag{502}$$

This is the same result than the equation $(S17)$, so we have proved that our general master equation allows to reproduce the results of the weak-coupling time-dependent. Now the master equation in the evolution time is given by

$$\frac{d\rho_S(t)}{dt} = -i\frac{\Omega\left(t\right)}{2}\left[\sigma_x, \rho_S\left(t\right)\right] - \frac{\pi}{8}J\left(\Omega\left(t\right)\right)\left(\left(n\left(\Omega\left(t\right)\right)+1\right)\left[\sigma_z, \left(\sigma_z + i\sigma_y\right)\rho_S\left(t\right)\right] + n\left(\Omega\left(t\right)\right)\left[\sigma_z, \left(\sigma_z - i\sigma_y\right)\rho_S\left(t\right)\right]\right) \tag{503}$$

$$- \frac{\pi}{8}J\left(\Omega\left(t\right)\right)\left(\left(n\left(\Omega\left(t\right)\right)+1\right)\left[\rho_S\left(t\right)\left(\sigma_z + i\sigma_y\right), \sigma_z\right] + n\left(\Omega\left(t\right)\right)\left[\rho_S\left(t\right)\left(\sigma_z - i\sigma_y\right), \sigma_z\right]\right) \tag{504}$$

VI. TIME-DEPENDENT MULTI-SITE MODEL WITH ONE BATH COUPLING

Let's consider the following Hamiltonian for a system of d-levels (qudit). We start with a time-dependent Hamiltonian of the form:

$$H(t) = H_S(t) + H_I + H_B, \tag{505}$$

$$H_S(t) = \sum_{n=0} \varepsilon_n(t) |n\rangle\langle n| + \sum_{n \neq m} V_{nm}(t) |n\rangle\langle m|, \tag{506}$$

$$H_I = \left(\sum_{n=0} \mu_n(t) |n\rangle\langle n| \right) \left(\sum_{\mathbf{k}} g_{\mathbf{k}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}} \right) \right), \tag{507}$$

$$H_B = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}. \tag{508}$$

We will start with a system-bath coupling operator of the form $\sum_{n=0} \mu_n(t) |n\rangle\langle n|$.

A. Variational Transformation

We consider the following operator:

$$V = \left(\sum_{n=1} |n\rangle\langle n| \right) \left(\sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \left(b_{\mathbf{k}}^\dagger - b_{\mathbf{k}} \right) \right) \tag{509}$$

At first let's obtain e^V under the transformation (509), consider $\hat{\varphi} = \sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \left(b_{\mathbf{k}}^\dagger - b_{\mathbf{k}} \right)$:

$$e^V = e^{\sum_{n=1} |n\rangle\langle n|\hat{\varphi}} \tag{510}$$

$$= \mathbb{I} + \sum_{n=1} |n\rangle\langle n|\hat{\varphi} + \frac{\left(\sum_{n=1} |n\rangle\langle n|\hat{\varphi} \right)^2}{2!} + \dots \tag{511}$$

$$= \mathbb{I} + \sum_{n=1} |n\rangle\langle n|\hat{\varphi} + \frac{\sum_{n=1} |n\rangle\langle n|\hat{\varphi}^2}{2!} + \dots \tag{512}$$

$$= \mathbb{I} - \sum_{n=1} |n\rangle\langle n| + \sum_{n=1} |n\rangle\langle n| \left(\mathbb{I} + \hat{\varphi} + \frac{\hat{\varphi}^2}{2!} + \dots \right) \tag{513}$$

$$= |0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n|e^{\hat{\varphi}} \tag{514}$$

$$= |0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n|B_+ \tag{515}$$

Given that $\left[b_{\mathbf{k}'}^\dagger - b_{\mathbf{k}'}, b_{\mathbf{k}}^\dagger - b_{\mathbf{k}} \right] = 0$ if $\mathbf{k}' \neq \mathbf{k}$ then we can proof using the Zassenhaus formula and defining $D\left(\pm \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right) = e^{\pm \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \left(b_{\mathbf{k}}^\dagger - b_{\mathbf{k}} \right)}$ in the same way than (23):

$$e^{\sum_{\mathbf{k}} \pm \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \left(b_{\mathbf{k}}^\dagger - b_{\mathbf{k}} \right)} = \prod_{\mathbf{k}} e^{\pm \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \left(b_{\mathbf{k}}^\dagger - b_{\mathbf{k}} \right)} \tag{516}$$

$$= \prod_{\mathbf{k}} D\left(\pm \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right) \tag{517}$$

$$= B_\pm \tag{518}$$

As we can see $e^{-V} = |0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n|B_-$ because this form imposes that $e^{-V}e^V = \mathbb{I}$ and the inverse of a operator is unique. This allows us to write the canonical transformation in the following explicit way:

$$e^V A e^{-V} = \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_+ \right) A \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_- \right) \tag{519}$$

Now let's obtain the canonical transformation of the principal elements of the Hamiltonian (505):

$$\overline{|0\rangle\langle 0|} = \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_+ \right) |0\rangle\langle 0| \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_- \right), \tag{520}$$

$$= |0\rangle\langle 0|, \tag{521}$$

$$\overline{|m\rangle\langle n|} = \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_+ \right) |m\rangle\langle n| \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_- \right), \tag{522}$$

$$= |m\rangle\langle m| B_+ |m\rangle\langle n| n\rangle\langle n| B_-, \tag{523}$$

$$= |m\rangle\langle n|, \ m \neq 0, \ n \neq 0, \tag{524}$$

$$\overline{|0\rangle\langle m|} = \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_+ \right) |0\rangle\langle m| \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_- \right), \tag{525}$$

$$= |0\rangle\langle m| B_- \ m \neq 0, \tag{526}$$

$$\overline{|m\rangle\langle 0|} = \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_+ \right) |m\rangle\langle 0| \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_- \right) \tag{527}$$

$$= |0\rangle\langle m| B_+ \ m \neq 0, \tag{528}$$

$$\overline{\sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}} = \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_+ \right) \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_- \right) \tag{529}$$

$$= |0\rangle\langle 0| \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sum_{n=1} |n\rangle\langle n| \sum_{\mathbf{k}} \omega_{\mathbf{k}} B_+ b_{\mathbf{k}}^\dagger b_{\mathbf{k}} B_- \tag{530}$$

$$= |0\rangle\langle 0| \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sum_{n=1} |n\rangle\langle n| \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(B_+ b_{\mathbf{k}}^\dagger B_- \right) \left(B_+ b_{\mathbf{k}} B_- \right) \tag{531}$$

$$= |0\rangle\langle 0| \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sum_{n=1} |n\rangle\langle n| \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(b_{\mathbf{k}}^\dagger - \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right) \left(b_{\mathbf{k}} - \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right) \tag{532}$$

$$= |0\rangle\langle 0| \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sum_{n=1} |n\rangle\langle n| \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(b_{\mathbf{k}}^\dagger b_{\mathbf{k}} - \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}} \right) + \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right) \tag{533}$$

$$= \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sum_{n=1} |n\rangle\langle n| \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} - \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}} \right) \right) \tag{534}$$

$$= \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sum_{n=1} |n\rangle\langle n| \sum_{\mathbf{k}} \omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} - \sum_{n=1} |n\rangle\langle n| \omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}} \right) \tag{535}$$

The transformed Hamiltonians of the equations (506) to (508) written in terms of (520) to (535) are:

$$\overline{H_{\bar{S}}(t)} = \overline{\sum_{n=0} \varepsilon_n(t) |n\rangle\langle n| + \sum_{n\neq m} V_{nm}(t) |n\rangle\langle m|} \tag{536}$$

$$= \overline{\sum_{n=0} \varepsilon_n(t) |n\rangle\langle n|} + \overline{\sum_{n\neq m} V_{nm}(t) |n\rangle\langle m|} \tag{537}$$

$$= \sum_{n=0} \varepsilon_n(t) |n\rangle\langle n| + \overline{\sum_{n=1} (V_{0n}(t) |0\rangle\langle n| + V_{n0}(t) |n\rangle\langle 0|)} + \overline{\sum_{m.n\neq 0} V_{mn}(t) |m\rangle\langle n|} \tag{538}$$

$$= \sum_{n=0} \varepsilon_n(t) |n\rangle\langle n| + \sum_{n=1} \left(V_{0n}(t) \overline{|0\rangle\langle n|} + V_{n0}(t) \overline{|n\rangle\langle 0|}\right) + \sum_{m.n\neq 0} V_{mn}(t) \overline{|m\rangle\langle n|} \tag{539}$$

$$= \sum_{n=0} \varepsilon_n(t) |n\rangle\langle n| + \sum_{n=1} (V_{0n}(t) B_- |0\rangle\langle n| + V_{n0}(t) B_+ |n\rangle\langle 0|) + \sum_{m.n\neq 0} V_{mn}(t) |m\rangle\langle n| \tag{540}$$

$$= \sum_{n=0} \varepsilon_n(t) |n\rangle\langle n| + \sum_{n=1} (V_{0n}(t) |0\rangle\langle n| B_- + V_{n0}(t) |n\rangle\langle 0| B_+) + \sum_{m.n\neq 0} V_{mn}(t) |m\rangle\langle n| \tag{541}$$

$$\overline{H_I} = \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_+\right) \left(\left(\sum_{n=0} \mu_n(t) |n\rangle\langle n|\right) \left(\sum_{\mathbf{k}} g_{\mathbf{k}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right)\right)\right) \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_-\right) \tag{542}$$

$$= \left(\mu_0(t) |0\rangle\langle 0| + \sum_{n=1} \mu_n(t) |n\rangle\langle n| B_+\right) \left(\sum_{\mathbf{k}} g_{\mathbf{k}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right)\right) \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_-\right) \tag{543}$$

$$= \mu_0(t) |0\rangle\langle 0| \sum_{\mathbf{k}} g_{\mathbf{k}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) + \sum_{n=1} \mu_n(t) |n\rangle\langle n| \sum_{\mathbf{k}} g_{\mathbf{k}} B_+ \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) B_- \tag{544}$$

$$= \mu_0(t) |0\rangle\langle 0| \sum_{\mathbf{k}} g_{\mathbf{k}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) + \sum_{n=1} \mu_n(t) |n\rangle\langle n| \sum_{\mathbf{k}} g_{\mathbf{k}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}} - 2\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\right) \tag{545}$$

$$\overline{H_B} = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sum_{n=1} |n\rangle\langle n| \sum_{\mathbf{k}} \omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} - \sum_{n=1} |n\rangle\langle n| \omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) \tag{546}$$

Joining this terms allow us to write:

$$\overline{H} = \sum_{n=0} \varepsilon_n(t) |n\rangle\langle n| + \sum_{n=1} (V_{0n}(t) |0\rangle\langle n| B_- + V_{n0}(t) |n\rangle\langle 0| B_+) + \sum_{m.n\neq 0} V_{mn}(t) |m\rangle\langle n| \tag{547}$$

$$+ \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sum_{n=1} |n\rangle\langle n| \sum_{\mathbf{k}} \omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} - \sum_{n=1} |n\rangle\langle n| \omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) \tag{548}$$

$$+ \sum_{n=0} \mu_n(t) |n\rangle\langle n| \sum_{\mathbf{k}} g_{\mathbf{k}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) - \sum_{n=1} \mu_n(t) |n\rangle\langle n| \sum_{\mathbf{k}} 2g_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \tag{549}$$

$$= \sum_{n=0} \varepsilon_n(t) |n\rangle\langle n| + \sum_{n=1} (V_{0n}(t) |0\rangle\langle n| B_- + V_{n0}(t) |n\rangle\langle 0| B_+) + \sum_{m.n\neq 0} V_{mn}(t) |m\rangle\langle n| \tag{550}$$

$$+ \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sum_{n=1} |n\rangle\langle n| \sum_{\mathbf{k}} \left(\omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} - 2\mu_n(t) g_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\right) + \mu_0(t) |0\rangle\langle 0| \sum_{\mathbf{k}} g_{\mathbf{k}} \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) \tag{551}$$

$$+ \sum_{n=1} |n\rangle\langle n| \sum_{\mathbf{k}} \left(g_{\mathbf{k}} \mu_n(t) - \omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\right) \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) \tag{552}$$

Let's define the following functions:

$$R_n(t) = \sum_{\mathbf{k}} \left(\omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} - 2\mu_n(t) g_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\right) \tag{553}$$

$$= \sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \left(\omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} - 2\mu_n(t) g_{\mathbf{k}}\right) \tag{554}$$

$$B_{z,n}(t) = \sum_{\mathbf{k}} \left(g_{\mathbf{k}} \mu_n(t) - \omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\right) \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) \tag{555}$$

Using the previous functions we have that (552) can be re-written in the following way:

$$\overline{H} = \sum_{n=0} \varepsilon_n\left(t\right)|n\rangle\langle n| + \sum_{n=1}\left(V_{0n}\left(t\right)|0\rangle\langle n|B_- + V_{n0}\left(t\right)|n\rangle\langle 0|B_+\right) + \sum_{m.n\neq 0} V_{mn}\left(t\right)|m\rangle\langle n| \tag{556}$$

$$+ \sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sum_{n=1}R_n|n\rangle\langle n| + \sum_{n=1}B_{z,n}|n\rangle\langle n| + \mu_0\left(t\right)|0\rangle\langle 0|\sum_{\mathbf{k}}g_{\mathbf{k}}\left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) \tag{557}$$

Now in order to separate the elements of the hamiltonian (557) let's follow the references of the equations (236) and (225) to separate the hamiltonian like:

$$\overline{H_S\left(t\right)} = \sum_{n=0}\varepsilon_n\left(t\right)|n\rangle\langle n| + B\sum_{n=1}\left(V_{0n}\left(t\right)|0\rangle\langle n| + V_{n0}\left(t\right)|n\rangle\langle 0|\right) + \sum_{m.n\neq 0}V_{mn}\left(t\right)|m\rangle\langle n| + \sum_{n=1}R_n|n\rangle\langle n| \tag{558}$$

$$\overline{H_I} = \sum_{n=1}B_{z,n}|n\rangle\langle n| + \mu_0\left(t\right)|0\rangle\langle 0|\sum_{\mathbf{k}}g_{\mathbf{k}}\left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) + \sum_{n=1}\left(V_{0n}\left(t\right)|0\rangle\langle n|\left(B_- - B\right) + V_{n0}\left(t\right)|n\rangle\langle 0|\left(B_+ - B\right)\right), \tag{559}$$

$$\overline{H_B} = \sum_{\mathbf{k}}\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \tag{560}$$

Here B is given by (158) The transformed Hamiltonian can be written in function of the following set of hermitian operators:

$$\sigma_{nm,x} = |n\rangle\langle m| + |m\rangle\langle n| \tag{561}$$

$$\sigma_{nm,y} = \mathrm{i}\left(|n\rangle\langle m| - |m\rangle\langle n|\right) \tag{562}$$

$$B_x = \frac{B_+ + B_- - 2B}{2} \tag{563}$$

$$B_y = \frac{B_- - B_+}{2\mathrm{i}} \tag{564}$$

Using this set of hermitian operators to write the Hamiltonians (506)-(508)

$$\overline{H_S(t)} = \varepsilon_0(t)\,|0\rangle\langle 0| + \sum_{n=1}(\varepsilon_n(t) + R_n)\,|n\rangle\langle n| + B\sum_{n=1}(V_{0n}(t)\,|0\rangle\langle n| + V_{n0}(t)\,|n\rangle\langle 0|) + \sum_{m.n\neq 0} V_{mn}(t)\,|m\rangle\langle n| \tag{565}$$

$$= \varepsilon_0(t)\,|0\rangle\langle 0| + B\sum_{n=1}(V_{0n}(t)\,|0\rangle\langle n| + V_{n0}(t)\,|n\rangle\langle 0|) + \sum_{0<m<n}(V_{mn}(t)\,|m\rangle\langle n| + V_{nm}(t)\,|n\rangle\langle m|) \tag{566}$$

$$+ \sum_{n=1}(\varepsilon_n(t) + R_n)\,|n\rangle\langle n| \tag{567}$$

$$= \sum_{0<m<n}\left((\Re(V_{mn}(t)) + \mathrm{i}\Im(V_{mn}(t)))\,|m\rangle\langle n| + (\Re(V_{mn}(t)) - \mathrm{i}\Im(V_{mn}(t)))\,|n\rangle\langle m|\right) + \varepsilon_0(t)\,|0\rangle\langle 0| \tag{568}$$

$$+ B\sum_{n=1}(V_{0n}(t)\,|0\rangle\langle n| + V_{n0}(t)\,|n\rangle\langle 0|) + \sum_{n=1}(\varepsilon_n(t) + R_n)\,|n\rangle\langle n| \tag{569}$$

$$= \sum_{0<m<n}\left((\Re(V_{nm}(t)) + \mathrm{i}\Im(V_{mn}(t)))\frac{\sigma_{nm,x} - \mathrm{i}\sigma_{nm,y}}{2} + (\Re(V_{nm}(t)) - \mathrm{i}\Im(V_{mn}(t)))\frac{\sigma_{nm,x} + \mathrm{i}\sigma_{nm,y}}{2}\right) \tag{570}$$

$$+ B\sum_{n=1}\left(V_{0n}(t)\frac{\sigma_{0n,x} - \mathrm{i}\sigma_{0n,y}}{2} + V_{n0}(t)\frac{\sigma_{0n,x} + \mathrm{i}\sigma_{0n,y}}{2}\right) + \varepsilon_0(t)\,|0\rangle\langle 0| + \sum_{n=1}(\varepsilon_n(t) + R_n)\,|n\rangle\langle n| \tag{571}$$

$$= \sum_{0<m<n}(\Re(V_{nm}(t))\,\sigma_{nm,x} + \Im(V_{nm}(t))\,\sigma_{nm,y}) + B\sum_{n=1}(\Re(V_{0n}(t))\,\sigma_{0n,x} + \Im(V_{mn}(t))\,\sigma_{0n,y}) \tag{572}$$

$$+ \varepsilon_0(t)\,|0\rangle\langle 0| + \sum_{n=1}(\varepsilon_n(t) + R_n)\,|n\rangle\langle n| \tag{573}$$

$$\overline{H_I(t)} = \sum_{n=1}B_{z,n}|n\rangle\langle n| + \mu_0(t)\,|0\rangle\langle 0|\sum_{\mathbf{k}}g_{\mathbf{k}}\left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) + \sum_{n=1}(V_{0n}(t)\,|0\rangle\langle n|(B_- - B) + V_{n0}(t)\,|n\rangle\langle 0|(B_+ - B)) \tag{574}$$

$$= \sum_{n=1}\left((\Re(V_{0n}(t)) + \mathrm{i}\Im(V_{0n}(t)))(B_- - B)\frac{\sigma_{0n,x} - \mathrm{i}\sigma_{0n,y}}{2} + (\Re(V_{0n}(t)) - \mathrm{i}\Im(V_{0n}(t)))(B_+ - B)\frac{\sigma_{0n,x} + \mathrm{i}\sigma_{0n,y}}{2}\right) \tag{575}$$

$$+ \sum_{n=1}B_{z,n}|n\rangle\langle n| + \mu_0(t)\,|0\rangle\langle 0|\sum_{\mathbf{k}}g_{\mathbf{k}}\left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) \tag{576}$$

$$= \sum_{n=1}B_{z,n}|n\rangle\langle n| + \sum_{n=1}\left(\frac{\sigma_{0n,x}}{2}((B_- - B)(\Re(V_{0n}(t)) + \mathrm{i}\Im(V_{0n}(t))) + (B_+ - B)(\Re(V_{0n}(t)) - \mathrm{i}\Im(V_{0n}(t))))\right. \tag{577}$$

$$\left.+ \frac{\mathrm{i}\sigma_{0n,y}}{2}((B_+ - B)(\Re(V_{0n}(t)) - \mathrm{i}\Im(V_{0n}(t))) - (B_- - B)(\Re(V_{0n}(t)) + \mathrm{i}\Im(V_{0n}(t))))\right) \tag{578}$$

$$+ \mu_0(t)\,|0\rangle\langle 0|\sum_{\mathbf{k}}g_{\mathbf{k}}\left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) \tag{579}$$

$$= \mu_0(t)\,|0\rangle\langle 0|\sum_{\mathbf{k}}g_{\mathbf{k}}\left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) + \sum_{n=1}\left(\frac{\sigma_{0n,x}}{2}(B_+ + B_- - 2B)\Re(V_{0n}(t)) + \mathrm{i}(B_- - B - B_+ + B)\Im(V_{0n}(t))\right. \tag{580}$$

$$\left.+ \frac{\mathrm{i}\sigma_{0n,y}}{2}((B_+ - B - B_- + B)\Re(V_{0n}(t)) + \mathrm{i}(B - B_- + B - B_+)\Im(V_{0n}(t)))\right) + \sum_{n=1}B_{z,n}|n\rangle\langle n| \tag{581}$$

$$= \sum_{n=1}B_{z,n}|n\rangle\langle n| + \mu_0(t)\,|0\rangle\langle 0|\sum_{\mathbf{k}}g_{\mathbf{k}}\left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) + \sum_{n=1}(\sigma_{0n,x}(B_x\Re(V_{0n}(t)) - B_y\Im(V_{0n}(t)))) \tag{582}$$

$$+ \sigma_{0n,y}(B_y\Re(V_{0n}(t)) + B_x\Im(V_{0n}(t)))) \tag{583}$$

B. Free-energy minimization

As first approach let's consider the minimization of the free-energy through the Feynman-Bogoliubov inequality

$$A \le A_{\mathrm{B}} \equiv -\frac{1}{\beta}\ln\left(\mathrm{Tr}\left(e^{-\beta(\overline{H_S + H_B})}\right)\right) + \langle \overline{H_I}\rangle_{H_S + H_B} + O\left(\langle \overline{H_I^2}\rangle_{H_S + H_B}\right). \tag{584}$$

Taking the equations (242)-(250) and given that $\mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right) = C\left(R_1, R_2, ..., R_{d-1}, B\right)$, where each R_i and B depend of the set of variational parameters $\{v_{\mathbf{k}}\}$. From (250) and using the chain rule we obtain that:

$$\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial v_{\mathbf{k}}} = \frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial B}\frac{\partial B}{\partial v_{\mathbf{k}}} + \sum_{n=1}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial R_n}\frac{\partial R_n}{\partial v_{\mathbf{k}}}, \tag{585}$$

$$= 0 \tag{586}$$

Let's recall the equations (553) and (555), we can write them in terms of the variational parameters

$$B = \exp\left(-(1/2)\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}^2}\coth\left(\beta\omega_{\mathbf{k}}/2\right)\right) \tag{587}$$

$$R_n = \sum_{\mathbf{k}}\omega_{\mathbf{k}}^{-1}\left(v_{\mathbf{k}} - 2\mu_n\left(t\right)g_{\mathbf{k}}v_{\mathbf{k}}\right) \tag{588}$$

The derivates needed to obtain the set of variational parameter are given by:

$$\frac{\partial B}{\partial v_{\mathbf{k}}} = -\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}^2}\coth\left(\beta\omega_{\mathbf{k}}/2\right)B \tag{589}$$

$$\frac{\partial R_n}{\partial v_{\mathbf{k}}} = \omega_{\mathbf{k}}^{-1}\left(2v_{\mathbf{k}} - 2\mu_n\left(t\right)g_{\mathbf{k}}\right) \tag{590}$$

Introducing this derivates in the equation (585) give us:

$$\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial v_{\mathbf{k}}} = \frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial B}\left(-\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}^2}\coth\left(\beta\omega_{\mathbf{k}}/2\right)B\right) + \sum_{n=1}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial R_n}\omega_{\mathbf{k}}^{-1}\left(2v_{\mathbf{k}} - 2\mu_n\left(t\right)g_{\mathbf{k}}\right) \tag{591}$$

$$= v_{\mathbf{k}}\left(\frac{2}{\omega_{\mathbf{k}}}\sum_{n=1}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial R_n} - \frac{\coth\left(\beta\omega_{\mathbf{k}}/2\right)B}{\omega_{\mathbf{k}}^2}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial B}\right) - \frac{2g_{\mathbf{k}}}{\omega_{\mathbf{k}}}\sum_{n=1}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial R_n}\mu_n\left(t\right) \tag{592}$$

We can obtain the variational parameters:

$$v_{\mathbf{k}} = \frac{\frac{2g_{\mathbf{k}}}{\omega_{\mathbf{k}}}\sum_{n=1}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial R_n}\mu_n\left(t\right)}{\frac{2}{\omega_{\mathbf{k}}}\sum_{n=1}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial R_n} - \frac{\coth(\beta\omega_{\mathbf{k}}/2)B}{\omega_{\mathbf{k}}^2}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial B}} \tag{593}$$

$$= \frac{2g_{\mathbf{k}}\omega_{\mathbf{k}}\sum_{n=1}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial R_n}\mu_n\left(t\right)}{2\omega_{\mathbf{k}}\sum_{n=1}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial R_n} - B\coth\left(\beta\omega_{\mathbf{k}}/2\right)\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial B}} \tag{594}$$

Now taking $v_{\mathbf{k}} = g_{\mathbf{k}}v_{\mathbf{k}}$ then we can obtain $v_{\mathbf{k}}$ like:

$$v_{\mathbf{k}} = \frac{2\omega_{\mathbf{k}}\sum_{n=1}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial R_n}\mu_n\left(t\right)}{2\omega_{\mathbf{k}}\sum_{n=1}\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial R_n} - B\coth\left(\beta\omega_{\mathbf{k}}/2\right)\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S}(t)}\right)}{\partial B}}. \tag{595}$$

C. Master Equation

Let's consider that the initial state of the system is given by $\rho(0) = |0\rangle\langle 0| \otimes \rho_B$, as we can see this state is independent of the variational transformation:

$$e^V \rho(0) e^{-V} = \left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_+\right)(|0\rangle\langle 0| \otimes \rho_B)\left(|0\rangle\langle 0| + \sum_{n=1} |n\rangle\langle n| B_-\right) \tag{596}$$

$$0 = |0\rangle\langle 0| \otimes \rho_B \tag{597}$$

$$0 = \rho(0) \tag{598}$$

We transform any operator O into the interaction picture in the following way:

$$\widetilde{O} \equiv U^\dagger(t) O U(t) \tag{599}$$

$$U(t) \equiv \mathcal{T} \exp\left(-i \int_0^t dv \overline{H_S}(v)\right). \tag{600}$$

Therefore:

$$\widetilde{\overline{\rho_S}}(t) = U^\dagger(t) \overline{\rho_S}(t) U(t), \text{ where} \tag{601}$$

$$\overline{\rho_S}(t) = \text{Tr}_B(\bar{\rho}(t)) \tag{602}$$

We can re-write the transformed interaction Hamiltonian operator like:

$$\overline{H_I(t)} = B_{z,0}|0\rangle\langle 0| + \sum_{n=1}\left(\Re(V_{0n}(t)) B_x \sigma_{0n,x} + \Re(V_{0n}(t)) B_y \sigma_{0n,y} + B_{z,n}|n\rangle\langle n|\right) \tag{603}$$

$$+ \Im(V_{0n}(t)) B_x \sigma_{0n,y} - \Im(V_{0n}(t)) B_y \sigma_{0n,x} \tag{604}$$

where

$$B_{z,0} = \sum_{\mathbf{k}} g_{\mathbf{k}} \mu_0(t) \left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) \tag{605}$$

$$B_{z,n} = \sum_{\mathbf{k}} \left(g_{\mathbf{k}} \mu_n(t) - \omega_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\right)\left(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}\right) \text{ if } n \neq 0 \tag{606}$$

Now consider the following set of operators:

$$A_{1n}(t) = \sigma_{0n,x} \tag{607}$$
$$A_{2n}(t) = \sigma_{0n,y} \tag{608}$$
$$A_{3n}(t) = |n\rangle\langle n| \tag{609}$$
$$A_{4n}(t) = A_{2n}(t) \tag{610}$$
$$A_{5n}(t) = A_{1n}(t) \tag{611}$$
$$B_{1n}(t) = B_x \tag{612}$$
$$B_{2n}(t) = B_y \tag{613}$$
$$B_{3n}(t) = B_{z,n} \tag{614}$$
$$B_{4n}(t) = B_{1n}(t) \tag{615}$$
$$B_{5n}(t) = B_{2n}(t) \tag{616}$$
$$C_{10}(t) = 0 \tag{617}$$
$$C_{20}(t) = 0 \tag{618}$$
$$C_{40}(t) = 0 \tag{619}$$
$$C_{50}(t) = 0 \tag{620}$$
$$C_{30}(t) = 1 \tag{621}$$
$$C_{1n}(t) = \Re(V_{0n}(t)) \tag{622}$$
$$C_{2n}(t) = C_{1n}(t) \tag{623}$$
$$C_{3n}(t) = 1 \tag{624}$$
$$C_{4n}(t) = \Im(V_{0n}(t)) \tag{625}$$
$$C_{5n}(t) = -\Im(V_{0n}(t)) \tag{626}$$

The previous notation allows us to write the interaction Hamiltonian in $\overline{H_I}(t)$ as:

$$\overline{H_I} = \sum_{j\in J}\sum_{n=1} C_{jn}(t)\left(A_{jn}\otimes B_{jn}(t)\right) \tag{627}$$

Here $J = \{1, 2, 3, 4, 5\}$.

We write the interaction Hamiltonian transformed under (599) as:

$$\widetilde{H_I}(t) = \sum_{j\in J}\sum_{n=1} C_{jn}(t)\left(\widetilde{A_{jn}}(t)\otimes\widetilde{B_{jn}}(t)\right) \tag{628}$$

$$\widetilde{A_i}(t) = U^\dagger(t)A_i U(t) \tag{629}$$

$$\widetilde{B_i}(t) = e^{iH_B t}B_i(t)e^{-iH_B t} \tag{630}$$

Taking as reference state ρ_B and truncating at second order in $H_I(t)$), we obtain our master equation in the interaction picture:

$$\frac{d\widetilde{\rho_S}(t)}{dt} = -\int_0^t \mathrm{Tr}_B\left[\widetilde{H_I}(t),\left[\widetilde{H_I}(s),\widetilde{\rho_S}(t)\rho_B\right]\right]ds \tag{631}$$

Replacing the equation (628)in (631)we can obtain:

$$\frac{\mathrm{d}\widetilde{\rho_S}(t)}{\mathrm{d}t} = -\int_0^t \mathrm{Tr}_B \left[\widetilde{H_I}(t), \left[\widetilde{H_I}(s), \widetilde{\rho_S}(t)\rho_B \right] \right] \mathrm{d}s \tag{632}$$

$$= -\int_0^t \mathrm{Tr}_B \left[\sum_{j \in J} \sum_{n=1} C_{jn}(t) \left(\widetilde{A_{jn}}(t) \otimes \widetilde{B_{jn}}(t) \right), \left[\sum_{j' \in J} \sum_{n'=1} C_{j'n'}(s) \left(\widetilde{A_{j'n'}}(s) \otimes \widetilde{B_{j'n'}}(s) \right), \widetilde{\rho_S}(t)\rho_B \right] \right] \mathrm{d}s \tag{633}$$

$$= -\int_0^t \mathrm{Tr}_B \left[\sum_{j \in J} \sum_{n=1} C_{jn}(t) \left(\widetilde{A_{jn}}(t) \otimes \widetilde{B_{jn}}(t) \right), \sum_{j' \in J} \sum_{n'=1} C_{j'n'}(s) \left(\widetilde{A_{j'n'}}(s) \otimes \widetilde{B_{j'n'}}(s) \right) \widetilde{\rho_S}(t)\rho_B \right. \tag{634}$$

$$\left. -\widetilde{\rho_S}(t)\rho_B \sum_{j' \in J} \sum_{n'=1} C_{j'n'}(s) \left(\widetilde{A_{j'n'}}(s) \otimes \widetilde{B_{j'n'}}(s) \right) \right] \mathrm{d}s \tag{635}$$

$$= -\int_0^t \mathrm{Tr}_B \left(\sum_{j \in J} \sum_{n=1} C_{jn}(t) \left(\widetilde{A_{jn}}(t) \otimes \widetilde{B_{jn}}(t) \right) \sum_{j' \in J} \sum_{n'=1} C_{j'n'}(s) \left(\widetilde{A_{j'n'}}(s) \otimes \widetilde{B_{j'n'}}(s) \right) \widetilde{\rho_S}(t)\rho_B \right. \tag{636}$$

$$-\sum_{j \in J} \sum_{n=1} C_{jn}(t) \left(\widetilde{A_{jn}}(t) \otimes \widetilde{B_{jn}}(t) \right) \widetilde{\rho_S}(t)\rho_B \sum_{j' \in J} \sum_{n'=1} C_{j'n'}(s) \left(\widetilde{A_{j'n'}}(s) \otimes \widetilde{B_{j'n'}}(s) \right) \tag{637}$$

$$-\sum_{j' \in J} \sum_{n'=1} C_{j'n'}(s) \left(\widetilde{A_{j'n'}}(s) \otimes \widetilde{B_{j'n'}}(s) \right) \widetilde{\rho_S}(t)\rho_B \sum_{j \in J} \sum_{n=1} C_{jn}(t) \left(\widetilde{A_{jn}}(t) \otimes \widetilde{B_{jn}}(t) \right) \tag{638}$$

$$+\widetilde{\rho_S}(t)\rho_B \sum_{j' \in J} \sum_{n'=1} C_{j'n'}(s) \left(\widetilde{A_{j'n'}}(s) \otimes \widetilde{B_{j'n'}}(s) \right) \sum_{j \in J} \sum_{n=1} C_{jn}(t) \left(\widetilde{A_{jn}}(t) \otimes \widetilde{B_{jn}}(t) \right) \right) \mathrm{d}s \tag{639}$$

In order to calculate the correlation functions we define:

$$\Lambda_{jnj'n'}(\tau) = \left\langle \widetilde{B_{jn}}(t)(t) \widetilde{B_{j'n'}}(t)(s) \right\rangle_B \tag{640}$$

$$= \left\langle \widetilde{B_{jn}}(\tau) \widetilde{B_{j'n'}}(0) \right\rangle_B \tag{641}$$

Here $s \to t - \tau$ and $\mathrm{Tr}_B \left(\widetilde{B_{jn}}(t) \widetilde{B_{j'n'}}(s) \rho_B \right) = \left\langle \widetilde{B_{jn}}(t) \widetilde{B_{j'n'}}(s) \right\rangle_B$. To evaluate the trace respect to the bath we need to recall that our master equation depends of elements related to the bath and represented by the operators $\widetilde{B_{jn}}(t)$ and elements related to the system given by $\widetilde{A_{jn}}(t)$. The systems considered are in different Hilbert spaces so $\mathrm{Tr} \left(\widetilde{A_{jn}}(t) \widetilde{B_{j'n'}}(t) \right) = \mathrm{Tr} \left(\widetilde{A_{jn}}(t) \right) \mathrm{Tr} \left(\widetilde{B_{j'n'}}(t) \right)$. The correlation functions relevant of the master equation (639) are:

$$\text{Tr}_B \left(\widetilde{B_{jn}}(t) \widetilde{B_{j'n'}}(s) \rho_B \right) = \left\langle \widetilde{B_{jn}}(t) \widetilde{B_{j'n'}}(s) \right\rangle_B \tag{642}$$

$$= \left\langle \widetilde{B_{jn}}(0) \widetilde{B_{j'n'}}(0) \right\rangle_B \tag{643}$$

$$= \Lambda_{jnj'n'}(\tau) \tag{644}$$

$$\text{Tr}_B \left(\widetilde{B_{jn}}(t) \rho_B \widetilde{B_{j'n'}}(s) \right) = \text{Tr}_B \left(\widetilde{B_{j'n'}}(s) \widetilde{B_{jn}}(t) \rho_B \right) \tag{645}$$

$$= \left\langle \widetilde{B_{j'n'}}(s) \widetilde{B_{jn}}(t) \right\rangle_B \tag{646}$$

$$= \left\langle \widetilde{B_{j'n'}}(-\tau) \widetilde{B_{jn}}(0) \right\rangle_B \tag{647}$$

$$= \Lambda_{j'n'jn}(-\tau) \tag{648}$$

$$\text{Tr}_B \left(\widetilde{B_{j'n'}}(s) \rho_B \widetilde{B_{jn}}(t) \right) = \text{Tr}_B \left(\widetilde{B_{jn}}(t) \widetilde{B_{j'n'}}(s) \rho_B \right) \tag{649}$$

$$= \left\langle \widetilde{B_{jn}}(t) \widetilde{B_{j'n'}}(s) \right\rangle_B \tag{650}$$

$$= \left\langle \widetilde{B_{jn}}(\tau) \widetilde{B_{j'n'}}(0) \right\rangle_B \tag{651}$$

$$= \Lambda_{jnj'n'}(\tau) \tag{652}$$

$$\text{Tr}_B \left(\rho_B \widetilde{B_{j'n'}}(s) \widetilde{B_{jn}}(t) \right) = \text{Tr}_B \left(\widetilde{B_{j'n'}}(s) \widetilde{B_{jn}}(t) \rho_B \right) \tag{653}$$

$$= \left\langle \widetilde{B_{j'n'}}(s) \widetilde{B_{jn}}(t) \right\rangle_B \tag{654}$$

$$= \left\langle \widetilde{B_{j'n'}}(-\tau) \widetilde{B_{jn}}(0) \right\rangle_B \tag{655}$$

$$= \Lambda_{j'n'jn}(-\tau) \tag{656}$$

We made use of the cyclic property for the trace to evaluate the correlation functions, from the equations obtained in (632)and (639) and using the equations (642)-(656) we can re-write:

$$\frac{d\widetilde{\rho_S}(t)}{dt} = -\int_0^t \sum_{j,j',n,n'} \left(C_{jn}(t) C_{j'n'}(s) \left(\Lambda_{jnj'n'}(\tau) \widetilde{A_{jn}}(t) \widetilde{A_{j'n'}}(s) \widetilde{\rho_S}(t) - \Lambda_{j'n'jn}(-\tau) \widetilde{A_{jn}}(t) \widetilde{\rho_S}(t) \widetilde{A_{j'n'}}(s) \right) \right. \tag{657}$$

$$\left. + C_{jn}(t) C_{j'n'}(s) \left(\Lambda_{j'n'jn}(-\tau) \widetilde{\rho_S}(t) \widetilde{A_{j'n'}}(s) \widetilde{A_{jn}}(t) - \Lambda_{jnj'n'}(\tau) \widetilde{A_{j'n'}}(s) \widetilde{\rho_S}(t) \widetilde{A_{jn}}(t) \right) \right) ds \tag{658}$$

$$= -\int_0^t \sum_{j,j',n,n'} \left(C_{jn}(t) C_{j'n'}(s) \left(\Lambda_{jnj'n'}(\tau) \left[\widetilde{A_{jn}}(t), \widetilde{A_{j'n'}}(s) \widetilde{\rho_S}(t) \right] + \Lambda_{j'n'jn}(-\tau) \left[\widetilde{\rho_S}(t) \widetilde{A_{j'n'}}(s), \widetilde{A_{jn}}(t) \right] \right) \right) \tag{659}$$

$$\frac{d \overline{\rho_S}(t)}{dt} = -\int_0^t \sum_{j,j',n,n'} \left(C_{jn}(t) C_{j'n'}(t-\tau) \left(\Lambda_{jnj'n'}(\tau) \left[A_{jn}(t), A_{j'n'}(t-\tau,t) \overline{\rho_S}(t) \right] + \Lambda_{j'n'jn}(-\tau) \left[\overline{\rho_S}(t) A_{j'n'}(t-\tau,t), A_{jn}(t) \right] \right) \right) d\tau - i \left[H_S(t), \overline{\rho_S}(t) \right] \tag{660}$$

For this case we used that $A_{jn}(t-\tau,t) = U(t) U^\dagger(t-\tau) A_{jn}(t) U(t-\tau) U^\dagger(t)$. This is a non-Markovian equation and if we take $n=2$ (two sites), $\mu_0(t) = 0$, $\mu_1(t) = 1$ then we can reproduce a similar expression to (350) as expected.

VII. TIME-DEPENDENT MULTI-SITE MODEL WITH V BATHS COUPLING

Let's consider the following Hamiltonian for a system of m-level system coupled to v-baths. We start with a time-dependent Hamiltonian of the form:

$$H(t) = H_S(t) + H_I + H_B, \tag{661}$$

$$H_S(t) = \sum_n \varepsilon_n(t) |n\rangle\langle n| + \sum_{n \neq m} V_{nm}(t) |n\rangle\langle m|, \tag{662}$$

$$H_I = \sum_{n,v,\mathbf{k}} \mu_{n,v}(t) |n\rangle\langle n| \left(g_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger + g_{v,\mathbf{k}}^* b_{v,\mathbf{k}} \right), \tag{663}$$

$$H_B = \sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}}. \tag{664}$$

A.   Variational Transformation

We consider the following operator:

$$V = \sum_{n,v,\mathbf{k}} a_{nv} |n\rangle\langle n| \omega_{v,\mathbf{k}}^{-1} \left(f_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger - f_{v,\mathbf{k}}^* b_{v,\mathbf{k}} \right) \tag{665}$$

We define $a_{nv} = 1$ if the site n is coupled to the bath v and $a_{nv} = 0$ in the other case. It allows to connect the variational transform of a given bath to the set of sites that relate with it.

At first let's obtain e^V under the transformation (665), consider $\hat{\varphi}_n = \sum_{v,\mathbf{k}} a_{nv} \omega_{v,\mathbf{k}}^{-1} \left(f_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger - f_{v,\mathbf{k}}^* b_{v,\mathbf{k}} \right)$, so the equation (665) can be written as $V = \sum_n |n\rangle\langle n| \hat{\varphi}_n$, then we have:

$$e^V = e^{\sum_n |n\rangle\langle n| \hat{\varphi}_n} \tag{666}$$

$$= \mathbb{I} + \sum_n |n\rangle\langle n| \hat{\varphi}_n + \frac{\left(\sum_n |n\rangle\langle n| \hat{\varphi}_n \right)^2}{2!} + \dots \tag{667}$$

$$= \mathbb{I} + \sum_n |n\rangle\langle n| \hat{\varphi}_n + \frac{\sum_n |n\rangle\langle n| \hat{\varphi}_n^2}{2!} + \dots \tag{668}$$

$$= \sum_n |n\rangle\langle n| + \sum_n |n\rangle\langle n| \hat{\varphi}_n + \frac{\sum_n |n\rangle\langle n| \hat{\varphi}_n^2}{2!} + \dots \tag{669}$$

$$= \sum_n |n\rangle\langle n| \left(\mathbb{I} + \hat{\varphi}_n + \frac{\hat{\varphi}_n^2}{2!} + \dots \right) \tag{670}$$

$$= \sum_n |n\rangle\langle n| e^{\hat{\varphi}_n} \tag{671}$$

Given that $\left[f_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger - f_{v,\mathbf{k}}^* b_{v,\mathbf{k}}, f_{v,\mathbf{k}'} b_{v,\mathbf{k}'}^\dagger - f_{v,\mathbf{k}'}^* b_{v,\mathbf{k}'} \right] = 0$ for all $\mathbf{k}'$, $\mathbf{k}$ then we can proof using the Zassenhaus formula and defining $D\left(\pm \alpha_{v,\mathbf{k}} \right) = e^{\pm \left(\alpha_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger - \alpha_{v,\mathbf{k}}^* b_{v,\mathbf{k}} \right)}$ in the same way than (23):

$$e^{\pm \sum_{v,\mathbf{k}} a_{nv} \left(\alpha_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger - \alpha_{v,\mathbf{k}}^* b_{v,\mathbf{k}} \right)} = \prod_v e^{\pm \sum_{\mathbf{k}} a_{nv} \left(\alpha_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger - \alpha_{v,\mathbf{k}}^* b_{v,\mathbf{k}} \right)} \tag{672}$$

$$= \prod_v \left(\prod_{\mathbf{k}} D\left(\pm \alpha_{v,\mathbf{k}} \right) \right)^{a_{nv}} \tag{673}$$

$$= \prod_v B_{v\pm}^{a_{nv}} \tag{674}$$

As we can see $e^{-V} = \sum_n |n\rangle\langle n| \prod_v B_{v-}^{a_{nv}}$ and $e^V = \sum_n |n\rangle\langle n| \prod_v B_{v+}^{a_{nv}}$ because this form imposes that $e^{-V} e^V = \mathbb{I}$ and the inverse of an operator is unique. This allows us to write the canonical transformation in the following explicit way:

$$e^V A e^{-V} = \left(\sum_n |n\rangle\langle n| \prod_v B_{v+}^{a_{nv}} \right) A \left(\sum_n |n\rangle\langle n| \prod_v B_{v-}^{a_{nv}} \right) \tag{675}$$

Now let's obtain the canonical transformation of the principal elements of the Hamiltonian (661):

$$\overline{|0\rangle\langle 0|} = \left(\sum_n |n\rangle\langle n| \prod_v B_{v+}^{a_{nv}} \right) |0\rangle\langle 0| \left(\sum_n |n\rangle\langle n| \prod_v B_{v-}^{a_{nv}} \right), \tag{676}$$

$$= \prod_v B_{v+}^{a_{0v}} |0\rangle\langle 0|0\rangle\langle 0|0\rangle\langle 0| \prod_v B_{v-}^{a_{0v}}, \tag{677}$$

$$= |0\rangle\langle 0| \prod_v B_{v+}^{a_{0v}} \prod_v B_{v-}^{a_{0v}}, \tag{678}$$

$$= |0\rangle\langle 0|. \tag{679}$$

$$\overline{|m\rangle\langle n|} = \left(\sum_n |n\rangle\langle n| \prod_v B_{v+}^{a_{nv}} \right) |m\rangle\langle n| \left(\sum_n |n\rangle\langle n| \prod_v B_{v-}^{a_{nv}} \right), \tag{680}$$

$$= |m\rangle\langle m| \prod_v B_{v+}^{a_{mv}} |m\rangle\langle n|n\rangle\langle n| \prod_v B_{v-}^{a_{nv}}, \tag{681}$$

$$= |m\rangle\langle n| \prod_v B_{v+}^{a_{mv}} \prod_v B_{v-}^{a_{nv}}, \; m \neq n, \tag{682}$$

$$\overline{\sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}}} = \left(\sum_n |n\rangle\langle n| \prod_v B_{v+}^{a_{nv}} \right) \sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}} \left(\sum_n |n\rangle\langle n| \prod_v B_{v-}^{a_{nv}} \right) \tag{683}$$

$$= \left(|0\rangle\langle 0| \prod_v B_{v+}^{a_{0v}} + |1\rangle\langle 1| \prod_v B_{v+}^{a_{1v}} + ... \right) \left(\sum_n |n\rangle\langle n| \sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}} \right) \left(|0\rangle\langle 0| \prod_v B_{v-}^{a_{0v}} + |1\rangle\langle 1| \prod_v B_{v-}^{a_{1v}} + ... \right) \tag{684}$$

$$= |0\rangle\langle 0| \prod_v B_{v+}^{a_{0v}} \sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}} \prod_v B_{v-}^{a_{0v}} + |1\rangle\langle 1| \prod_v B_{v+}^{a_{1v}} \sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}} \prod_v B_{v-}^{a_{1v}} + ... \tag{685}$$

$$= |0\rangle\langle 0| \prod_v B_{v+}^{a_{0v}} \left(\sum_\mathbf{k} \omega_{0,\mathbf{k}} b_{0,\mathbf{k}}^\dagger b_{0,\mathbf{k}} + \sum_\mathbf{k} \omega_{1,\mathbf{k}} b_{1,\mathbf{k}}^\dagger b_{1,\mathbf{k}} + ... \right) \prod_v B_{v-}^{a_{0v}} + ... \tag{686}$$

$$= |0\rangle\langle 0| \left(\prod_v B_{v+}^{a_{0v}} \sum_\mathbf{k} \omega_{0,\mathbf{k}} b_{0,\mathbf{k}}^\dagger b_{0,\mathbf{k}} \prod_v B_{v-}^{a_{0v}} + \prod_v B_{v+}^{a_{0v}} \sum_\mathbf{k} \omega_{1,\mathbf{k}} b_{1,\mathbf{k}}^\dagger b_{1,\mathbf{k}} \prod_v B_{v-}^{a_{0v}} + ... \right) + ... \tag{687}$$

$$= |0\rangle\langle 0| \left(\sum_\mathbf{k} \omega_{0,\mathbf{k}} \left(b_{0,\mathbf{k}}^\dagger - a_{00}\alpha_{0,\mathbf{k}}^* \right) \left(b_{0,\mathbf{k}} - a_{00}\alpha_{0,\mathbf{k}} \right) + \sum_\mathbf{k} \omega_{1,\mathbf{k}} \left(b_{1,\mathbf{k}}^\dagger - a_{01}\alpha_{1,\mathbf{k}}^* \right) \left(b_{1,\mathbf{k}} - a_{01}\alpha_{1,\mathbf{k}} \right) + ... \right) + ... \tag{688}$$

$$= |0\rangle\langle 0| \left(\sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}} \left(b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}} - a_{0v} \left(\alpha_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger + \alpha_{v,\mathbf{k}}^* b_{v,\mathbf{k}} \right) + a_{0v}^2 |\alpha_{v,\mathbf{k}}|^2 \right) \right) + ... \tag{689}$$

$$= |0\rangle\langle 0| \left(\sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}} + \sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}} \left(a_{0v}^2 |\alpha_{v,\mathbf{k}}|^2 - a_{0v} \left(\alpha_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger + \alpha_{v,\mathbf{k}}^* b_{v,\mathbf{k}} \right) \right) \right) + ... \tag{690}$$

$$= \sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}} + \sum_{n,v,\mathbf{k}} |n\rangle\langle n| \omega_{v,\mathbf{k}} \left(a_{nv}^2 |\alpha_{v,\mathbf{k}}|^2 - a_{nv} \left(\alpha_{v,\mathbf{k}} b_{v,\mathbf{k}}^\dagger + \alpha_{v,\mathbf{k}}^* b_{v,\mathbf{k}} \right) \right) \tag{691}$$

The transformed Hamiltonians of the equations (662) to (664) written in terms of (676) to (691) are:

$$\overline{H_S(t)} = \overline{\sum_n \varepsilon_n(t)\,|n\rangle\langle n| + \sum_{n\neq m} V_{nm}(t)\,|n\rangle\langle m|} \tag{692}$$

$$= \sum_n \varepsilon_n(t)\,|n\rangle\langle n| + \overline{\sum_{n\neq m} V_{nm}(t)\,|n\rangle\langle m|} \tag{693}$$

$$= \sum_n \varepsilon_n(t)\,|n\rangle\langle n| + \sum_{n\neq m} V_{nm}(t)\,|n\rangle\langle m| \prod_v B_{v+}^{a_{nv}} \prod_v B_{v-}^{a_{mv}} \tag{694}$$

$$\overline{H_I} = \left(\sum_n |n\rangle\langle n| \prod_v B_{v+}^{a_{nv}}\right)\left(\sum_{n,v,\mathbf{k}} \mu_{n,v}(t)\,|n\rangle\langle n| \left(g_{v,\mathbf{k}}b_{v,\mathbf{k}}^\dagger + g_{v,\mathbf{k}}^* b_{v,\mathbf{k}}\right)\right)\left(\sum_n |n\rangle\langle n| \prod_v B_{v-}^{a_{nv}}\right) \tag{695}$$

$$= \left(\sum_n |n\rangle\langle n| \prod_v B_{v+}^{a_{nv}}\right)\left(\sum_{v,\mathbf{k}} \mu_{0,v}(t)\,|0\rangle\langle 0| \left(g_{v,\mathbf{k}}b_{v,\mathbf{k}}^\dagger + g_{v,\mathbf{k}}^* b_{v,\mathbf{k}}\right) + ...\right)\left(\sum_n |n\rangle\langle n| \prod_v B_{v-}^{a_{nv}}\right) \tag{696}$$

$$= \prod_v B_{v+}^{a_{0v}} \sum_{v,\mathbf{k}} \mu_{0,v}(t)\,|0\rangle\langle 0| \left(g_{v,\mathbf{k}}b_{v,\mathbf{k}}^\dagger + g_{v,\mathbf{k}}^* b_{v,\mathbf{k}}\right)\prod_v B_{v-}^{a_{0v}} + ... \tag{697}$$

$$= \prod_v B_{v+}^{a_{0v}} \left(\sum_{\mathbf{k}} \mu_{0,0}(t)\,|0\rangle\langle 0| \left(g_{0,\mathbf{k}}b_{0,\mathbf{k}}^\dagger + g_{0,\mathbf{k}}^* b_{0,\mathbf{k}}\right) + ...\right)\prod_v B_{v-}^{a_{0v}} + ... \tag{698}$$

$$= \left(\sum_{\mathbf{k}} \mu_{0,0}(t)\,|0\rangle\langle 0| \left(g_{0,\mathbf{k}}\left(b_{0,\mathbf{k}}^\dagger - a_{00}\alpha_{0,\mathbf{k}}^*\right) + g_{0,\mathbf{k}}^*\left(b_{0,\mathbf{k}} - a_{00}\alpha_{0,\mathbf{k}}\right)\right) + ...\right) + ... \tag{699}$$

$$= \sum_{v,\mathbf{k}} \mu_{0,v}(t)\,|0\rangle\langle 0| \left(g_{v,\mathbf{k}}\left(b_{v,\mathbf{k}}^\dagger - a_{0v}\alpha_{v,\mathbf{k}}^*\right) + g_{v,\mathbf{k}}^*\left(b_{v,\mathbf{k}} - a_{0v}\alpha_{v,\mathbf{k}}\right)\right) + ... \tag{700}$$

$$= \sum_{n,v,\mathbf{k}} \mu_{n,v}(t)\,|n\rangle\langle n| \left(g_{v,\mathbf{k}}\left(b_{v,\mathbf{k}}^\dagger - a_{nv}\alpha_{v,\mathbf{k}}^*\right) + g_{v,\mathbf{k}}^*\left(b_{v,\mathbf{k}} - a_{nv}\alpha_{v,\mathbf{k}}\right)\right) \tag{701}$$

$$\overline{H_B} = \sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}}b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}} + \sum_{n,v,\mathbf{k}} |n\rangle\langle n| \omega_{v,\mathbf{k}}\left(a_{nv}^2|\alpha_{v,\mathbf{k}}|^2 - a_{nv}\left(\alpha_{v,\mathbf{k}}b_{v,\mathbf{k}}^\dagger + \alpha_{v,\mathbf{k}}^* b_{v,\mathbf{k}}\right)\right) \tag{702}$$

Joining this terms allow us to write the transformed Hamiltonian as:

$$\overline{H} = \sum_n \varepsilon_n(t)\,|n\rangle\langle n| + \sum_{n\neq m} V_{nm}(t)\,|n\rangle\langle m| \prod_v B_{v+}^{a_{nv}} \prod_v B_{v-}^{a_{mv}} + \sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}}b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}} + \sum_{n,v,\mathbf{k}} |n\rangle\langle n| \omega_{v,\mathbf{k}}\left(a_{nv}^2|\alpha_{v,\mathbf{k}}|^2\right. \tag{703}$$

$$\left. - a_{nv}\left(\alpha_{v,\mathbf{k}}b_{v,\mathbf{k}}^\dagger + \alpha_{v,\mathbf{k}}^* b_{v,\mathbf{k}}\right)\right) + \sum_{n,v,\mathbf{k}} \mu_{n,v}(t)\,|n\rangle\langle n| \left(g_{v,\mathbf{k}}\left(b_{v,\mathbf{k}}^\dagger - a_{nv}\alpha_{v,\mathbf{k}}^*\right) + g_{v,\mathbf{k}}^*\left(b_{v,\mathbf{k}} - a_{nv}\alpha_{v,\mathbf{k}}\right)\right) \tag{704}$$

Let's define the following functions, given that $a_{nv} = 0,1$ then $a_{nv} = a_{nv}^2$ so we can reduce it in the equations:

$$R_n(t) = \sum_{v,\mathbf{k}} a_{nv}\left(\omega_{v,\mathbf{k}}|\alpha_{v,\mathbf{k}}|^2 - \mu_{n,v}(t)\left(g_{v,\mathbf{k}}\alpha_{v,\mathbf{k}}^* + g_{v,\mathbf{k}}^*\alpha_{v,\mathbf{k}}\right)\right) \tag{705}$$

$$B_{z,n}(t) = \sum_{v,\mathbf{k}} \left(\mu_{n,v}(t)\left(g_{v,\mathbf{k}}b_{v,\mathbf{k}}^\dagger + g_{v,\mathbf{k}}^* b_{v,\mathbf{k}}\right) - \omega_{v,\mathbf{k}}a_{nv}\left(\alpha_{v,\mathbf{k}}b_{v,\mathbf{k}}^\dagger + \alpha_{v,\mathbf{k}}^* b_{v,\mathbf{k}}\right)\right) \tag{706}$$

Using the previous functions we have that (703) can be re-written in the following way:

$$\overline{H} = \sum_n \varepsilon_n(t)\,|n\rangle\langle n| + \sum_{n\neq m} V_{nm}(t)\,|n\rangle\langle m| \prod_v B_{v+}^{a_{nv}} \prod_v B_{v-}^{a_{mv}} + \sum_{v,\mathbf{k}} \omega_{v,\mathbf{k}}b_{v,\mathbf{k}}^\dagger b_{v,\mathbf{k}} \tag{707}$$

$$+ \sum_n R_n(t)\,|n\rangle\langle n| + \sum_n B_{z,n}(t)\,|n\rangle\langle n| \tag{708}$$

Now in order to separate the elements of the hamiltonian (708) let's follow the references of the equations (225) and (236) to separate the hamiltonian, before proceding to do this we need to consider the term of the form:

$$\langle B_{n+} B_{m-} \rangle_{\overline{H_0}} = \langle B_{n+} \rangle_{\overline{H_0}} \langle B_{m-} \rangle_{\overline{H_0}} \tag{709}$$

The previous expression is true because $n \neq m$, so it's possible to separate the expected values. In this context can deduce using (152)that:

$$B_n = \langle B_{n\pm} \rangle_{\overline{H_0}} \tag{710}$$

$$= \exp\left(-(1/2) \sum_{\mathbf{k}} \frac{f_{n,\mathbf{k}}^2}{\omega_{n,\mathbf{k}}^2} \coth\left(\beta \omega_{n,\mathbf{k}}/2 \right) \right) \tag{711}$$

Following the reference [4] we define:

$$B_{nm} = B_{n+} B_{m-} - B_n B_m \tag{712}$$

We can separate the Hamiltonian (708) on the following way using similar arguments to the previous cases in order to satisfy $\langle \overline{H_I} \rangle_{\overline{H_0}} = 0$:

$$\overline{H_S(t)} = \sum_n \left(\varepsilon_n(t) + R_n \right) |n\rangle\langle n| + \sum_{n \neq m} V_{nm}(t) |n\rangle\langle m| B_n B_m \tag{713}$$

$$\overline{H_I} = \sum_{n \neq m} V_{nm}(t) |n\rangle\langle m| B_{nm} + \sum_n B_{z,n}(t) |n\rangle\langle n|, \tag{714}$$

$$\overline{H_B} = \sum_{n,\mathbf{k}} \omega_{n,\mathbf{k}} b_{n,\mathbf{k}}^\dagger b_{n,\mathbf{k}} \tag{715}$$

B. Free-energy minimization

As first approach let's consider the minimization of the free-energy through the Feynman-Bogoliubov inequality

$$A \leq A_{\mathrm{B}} \equiv -\frac{1}{\beta} \ln\left(\mathrm{Tr}\left(e^{-\beta(\overline{H_S} + \overline{H_B})} \right) \right) + \langle \overline{H_I} \rangle_{\overline{H_S + H_B}} + O\left(\langle \overline{H_I^2} \rangle_{\overline{H_S + H_B}} \right). \tag{716}$$

Taking the equations (242)-(250) and given that $\mathrm{Tr}\left(e^{-\beta \overline{H_S(t)}} \right) = C\left(R_0, R_1, R_2, ..., R_{d-1}, B_0, B_1, B_2, ..., B_{d-1} \right)$, where each R_i and B_i depend of the set of variational parameters $\{ f_{n,\mathbf{k}} \}$ then we can obtain using the chain rule that:

$$\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S(t)}} \right)}{\partial f_{n,\mathbf{k}}} = \sum_{n'} \left(\frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S(t)}} \right)}{\partial B_{n'}} \frac{\partial B_{n'}}{\partial f_{n,\mathbf{k}}} + \frac{\partial \mathrm{Tr}\left(e^{-\beta \overline{H_S(t)}} \right)}{\partial R_{n'}} \frac{\partial R_{n'}}{\partial f_{n,\mathbf{k}}} \right) \tag{717}$$

$$= 0 \tag{718}$$

Let's recall the equations (705) and (706), we can write them in terms of the variational parameters

$$B_{n'} = \exp\left(-(1/2) \sum_{\mathbf{k}} \frac{f_{n',\mathbf{k}}^2}{\omega_{n',\mathbf{k}}^2} \coth\left(\beta \omega_{n',\mathbf{k}}/2 \right) \right) \tag{719}$$

$$R_{n'} = \sum_{\mathbf{k}} \omega_{n',\mathbf{k}} \alpha_{n',\mathbf{k}}^2 - 2 \sum_{v,\mathbf{k}} \mu_{n',v}(t) g_{n',\mathbf{k}} \alpha_{n',\mathbf{k}} \tag{720}$$

The derivates needed to obtain the set of variational parameter are given by:

$$\frac{\partial B_{n'}}{\partial f_{n,\mathbf{k}}} = -\frac{f_{n,\mathbf{k}}}{\omega_{n,\mathbf{k}}^2} \coth\left(\beta\omega_{n,\mathbf{k}}/2\right) B_n\, \delta_{f_{n,\mathbf{k}},f_{n',\mathbf{k}}} \tag{721}$$

$$\frac{\partial R_{n'}}{\partial f_{n,\mathbf{k}}} = \omega_{n,\mathbf{k}}^{-1}\left(2f_{n,\mathbf{k}} - 2\sum_v \mu_{n,v}(t)\, g_{n,\mathbf{k}}\right) \delta_{f_{n,\mathbf{k}},f_{n',\mathbf{k}}} \tag{722}$$

Introducing this derivates in the equation (717) give us:

$$\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial f_{n,\mathbf{k}}} = \sum_{n'} \frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial B_{n'}}\left(-\frac{f_{n,\mathbf{k}}}{\omega_{n,\mathbf{k}}^2}\coth\left(\beta\omega_{n,\mathbf{k}}/2\right)B_n\right)\delta_{f_{n,\mathbf{k}},f_{n',\mathbf{k}}} \tag{723}$$

$$+ \sum_{n'} \frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial R_n}\, \omega_{n,\mathbf{k}}^{-1}\left(2f_{n,\mathbf{k}} - 2\sum_v \mu_{n,v}(t)\, g_{n,\mathbf{k}}\right)\delta_{f_{n,\mathbf{k}},f_{n',\mathbf{k}}} \tag{724}$$

$$= f_{n,\mathbf{k}}\left(\sum_{n'}\left(\frac{2}{\omega_{n,\mathbf{k}}}\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial R_n} - \frac{\coth\left(\beta\omega_{n,\mathbf{k}}/2\right)B_n}{\omega_{n,\mathbf{k}}^2}\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial B_n}\right)\delta_{f_{n,\mathbf{k}},f_{n',\mathbf{k}}}\right) \tag{725}$$

$$- 2\sum_{n'}\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial R_n}\,\omega_{n,\mathbf{k}}^{-1}\sum_v \mu_{n,v}(t)\, g_{n,\mathbf{k}}\,\delta_{f_{n,\mathbf{k}},f_{n',\mathbf{k}}} \tag{726}$$

We can obtain the variational parameters:

$$f_{n,\mathbf{k}} = \frac{2\sum_{n'}\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial R_n}\,\omega_{n,\mathbf{k}}^{-1}\sum_v \mu_{n,v}(t)\, g_{n,\mathbf{k}}\,\delta_{f_{n,\mathbf{k}},f_{n',\mathbf{k}}}}{\sum_{n'}\left(\frac{2}{\omega_{n,\mathbf{k}}}\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial R_n} - \frac{\coth(\beta\omega_{n,\mathbf{k}}/2)B_n}{\omega_{n,\mathbf{k}}^2}\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial B_n}\right)\delta_{f_{n,\mathbf{k}},f_{n',\mathbf{k}}}} \tag{727}$$

$$= \frac{2\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial R_n}\,\omega_{n,\mathbf{k}}\sum_v \mu_{n,v}(t)\, g_{n,\mathbf{k}}}{\left(2\omega_{n,\mathbf{k}}\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial R_n} - \coth\left(\beta\omega_{n,\mathbf{k}}/2\right)B_n\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial B_n}\right)} \tag{728}$$

We reduced $\sum_{n'}\delta_{f_{n,\mathbf{k}},f_{n',\mathbf{k}}}$ in the numerator and denominator provided that this expression is not zero. Now taking $f_{n,\mathbf{k}} = g_{n,\mathbf{k}}F_{n,\mathbf{k}}$ then we can obtain $F_{n,\mathbf{k}}$ like:

$$F_{n,\mathbf{k}} = \frac{2\omega_{n,\mathbf{k}}\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial R_n}\sum_v \mu_{n,v}(t)}{\left(2\omega_{n,\mathbf{k}}\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial R_n} - \coth\left(\beta\omega_{n,\mathbf{k}}/2\right)B_n\frac{\partial \mathrm{Tr}\left(e^{-\beta\overline{H_S(t)}}\right)}{\partial B_n}\right)} \tag{729}$$

For the reference [4] we have that $\sum_v \mu_{n,v}(t) = 1$, so the variational parameters of this reference are a special case of the equation (729).

C. Master Equation

Let's consider that the initial state of the system is given by $\rho(0) = |0\rangle\langle0| \otimes \rho_B$, as we can see this state is independent of the variational transformation:

$$e^V \rho(0) e^{-V} = \left(\sum_n |n\rangle\langle n| B_{n+}\right)(|0\rangle\langle0| \otimes \rho_B)\left(\sum_n |n\rangle\langle n| B_{n+}\right) \tag{730}$$

$$0 = (B_{0+}|0\rangle\langle0|B_{0-}) \otimes \rho_B \tag{731}$$

$$0 = \rho(0) \tag{732}$$

We transform any operator O into the interaction picture in the following way:

$$\widetilde{O} \equiv U^\dagger(t)OU(t) \tag{733}$$

$$U(t) \equiv \mathcal{T}\exp\left(-\mathrm{i}\int_0^t \mathrm{d}v\overline{H_S}(v)\right). \tag{734}$$

Therefore:

$$\widetilde{\overline{\rho_S}}(t) = U^\dagger(t)\overline{\rho_S}(t)U(t), \text{ where} \tag{735}$$

$$\overline{\rho_S}(t) = \mathrm{Tr}_B(\bar{\rho}(t)) \tag{736}$$

We can re-write the transformed interaction Hamiltonian operator using the following matrices:

$$\sigma_{nm,x} = |n\rangle\langle m| + |m\rangle\langle n| \tag{737}$$

$$\sigma_{nm,y} = \mathrm{i}(|n\rangle\langle m| - |m\rangle\langle n|) \tag{738}$$

$$B_{nm,x} = \frac{B_{nm} + B_{mn}}{2} \tag{739}$$

$$B_{nm,x} = \frac{B_{nm} - B_{mn}}{2\mathrm{i}} \tag{740}$$

We can proof that $B_{nm} = B_{mn}^\dagger$

$$B_{mn}^\dagger = (B_{m+}B_{n-} - B_m B_n)^\dagger \tag{741}$$

$$= B_{n-}^\dagger B_{m+}^\dagger - B_n B_m \tag{742}$$

$$= B_{n+}B_{m-} - B_n B_m \tag{743}$$

$$= B_{nm} \tag{744}$$

So we can say that the set of matrices (737) are hermitic. Re-writing the transformed interaction hamiltonian using the set (737) give us.

$$\overline{H_I} = \sum_{n \neq m} V_{nm}(t)|n\rangle\langle m|B_{nm} + \sum_n B_{z,n}(t)|n\rangle\langle n|, \tag{745}$$

$$= \sum_n B_{z,n}(t)|n\rangle\langle n| + \sum_{n<m}(V_{nm}(t)|n\rangle\langle m|B_{nm} + V_{mn}(t)|m\rangle\langle n|B_{mn}) \tag{746}$$

$$= \sum_n B_{z,n}(t)|n\rangle\langle n| + \sum_{n<m}\left(\Re(V_{nm}(t))B_{nm}\left(\frac{\sigma_{nm,x} - \mathrm{i}\sigma_{nm,y}}{2}\right) + \mathrm{i}\Im(V_{nm}(t))B_{nm}\left(\frac{\sigma_{nm,x} - \mathrm{i}\sigma_{nm,y}}{2}\right)\right. \tag{747}$$

$$\left. +\Re(V_{nm}(t))B_{mn}\left(\frac{\sigma_{nm,x} + \mathrm{i}\sigma_{nm,y}}{2}\right) - \mathrm{i}\Im(V_{nm}(t))B_{mn}\left(\frac{\sigma_{nm,x} + \mathrm{i}\sigma_{nm,y}}{2}\right)\right) \tag{748}$$

$$= \sum_n B_{z,n}(t)|n\rangle\langle n| + \sum_{n<m}\left(\Re(V_{nm}(t))\sigma_{nm,x}\left(\frac{B_{nm} + B_{mn}}{2}\right) + \Re(V_{nm}(t))\sigma_{nm,y}\frac{\mathrm{i}(B_{mn} - B_{nm})}{2}\right. \tag{749}$$

$$\left. +\mathrm{i}\Im(V_{nm}(t))\sigma_{nm,x}\left(\frac{B_{nm} - B_{mn}}{2}\right) + \Im(V_{nm}(t))\sigma_{nm,y}\left(\frac{B_{nm} + B_{mn}}{2}\right)\right) \tag{750}$$

$$= \sum_n B_{z,n}(t)|n\rangle\langle n| + \sum_{n<m}(\Re(V_{nm}(t))\sigma_{nm,x}B_{nm,x} - \Im(V_{nm}(t))\sigma_{nm,x}B_{nm,y} + \Re(V_{nm}(t))\sigma_{nm,y}B_{nm,y} \tag{751}$$

$$+\Im(V_{nm}(t))\sigma_{nm,y}B_{nm,x}) \tag{752}$$

Let's define the set

$$P = \{(n,m) \in \mathbb{N}^2 | 0 \leq n, m \leq d-1 \wedge (n = m \vee n < m)\} \tag{753}$$

Now consider the following set of operators,

$$A_{1,nm}(t) = \sigma_{nm,x}(1 - \delta_{mn}) \tag{754}$$
$$A_{2,nm}(t) = \sigma_{nm,y}(1 - \delta_{mn}) \tag{755}$$
$$A_{3,nm}(t) = \delta_{mn}|n\rangle\langle m| \tag{756}$$
$$A_{4,nm}(t) = A_{2,mn}(t) \tag{757}$$
$$A_{5,nm}(t) = A_{1,nm}(t) \tag{758}$$
$$B_{1,nm}(t) = B_{nm,x} \tag{759}$$
$$B_{2,nm}(t) = B_{nm,y} \tag{760}$$
$$B_{3,nm}(t) = B_{z,n}(t) \tag{761}$$
$$B_{4,nm}(t) = B_{1,nm}(t) \tag{762}$$
$$B_{5,nm}(t) = B_{2,nm}(t) \tag{763}$$
$$C_{1,nm}(t) = \Re(V_{nm}(t)) \tag{764}$$
$$C_{2,nm}(t) = C_{1,nm}(t) \tag{765}$$
$$C_{3,nm}(t) = 1 \tag{766}$$
$$C_{4,nm}(t) = \Im(V_{nm}(t)) \tag{767}$$
$$C_{5,nm}(t) = -\Im(V_{nm}(t)) \tag{768}$$

The previous notation allows us to write the interaction Hamiltonian in $\overline{H_I}(t)$ as:

$$\overline{H_I} = \sum_{j \in J, p \in P} C_{jp}(t)(A_{jp} \otimes B_{jp}(t)) \tag{769}$$

Here $J = \{1,2,3,4,5\}$ and P the set defined in (753).

We write the interaction Hamiltonian transformed under (733) as:

$$\widetilde{H_I}(t) = \sum_{j \in J, p \in P} C_{jp}(t)\left(\widetilde{A_{jp}}(t) \otimes \widetilde{B_{jp}}(t)\right) \tag{770}$$

$$\widetilde{A_{jp}}(t) = U^{\dagger}(t) A_{jp} U(t) \tag{771}$$

$$\widetilde{B_{jp}}(t) = e^{iH_B t} B_{jp}(t)(t) e^{-iH_B t} \tag{772}$$

Taking as reference state ρ_B and truncating at second order in $H_I(t)$, we obtain our master equation in the interaction picture:

$$\frac{d\widetilde{\rho_S}(t)}{dt} = -\int_0^t \text{Tr}_B\left[\widetilde{H_I}(t), \left[\widetilde{H_I}(s), \widetilde{\rho_S}(t)\rho_B\right]\right] ds \tag{773}$$

Replacing the equation (770) in (773) we can obtain:

$$\frac{\mathrm{d}\widetilde{\rho_S}(t)}{\mathrm{d}t} = -\int_0^t \mathrm{Tr}_B\left[\widetilde{H_I}(t),\left[\widetilde{H_I}(s),\widetilde{\rho_S}(t)\rho_B\right]\right]\mathrm{d}s \tag{774}$$

$$= -\int_0^t \mathrm{Tr}_B\left[\sum_{j\in J,p\in P}C_{jp}(t)\left(\widetilde{A_{jp}}(t)\otimes\widetilde{B_{jp}}(t)\right),\left[\sum_{j'\in J,p'\in P}C_{j'p'}(s)\left(\widetilde{A_{j'p'}}(s)\otimes\widetilde{B_{j'p'}}(s)\right),\widetilde{\rho_S}(t)\rho_B\right]\right]\mathrm{d}s \tag{775}$$

$$= -\int_0^t \mathrm{Tr}_B\left[\sum_{j\in J,p\in P}C_{jp}(t)\left(\widetilde{A_{jp}}(t)\otimes\widetilde{B_{jp}}(t)\right),\sum_{j'\in J,p'\in P}C_{j'p'}(s)\left(\widetilde{A_{j'p'}}(s)\otimes\widetilde{B_{j'p'}}(s)\right)\widetilde{\rho_S}(t)\rho_B\right. \tag{776}$$

$$\left.-\widetilde{\rho_S}(t)\rho_B\sum_{j'\in J,p'\in P}C_{j'p'}(s)\left(\widetilde{A_{j'p'}}(s)\otimes\widetilde{B_{j'p'}}(s)\right)\right]\mathrm{d}s \tag{777}$$

$$= -\int_0^t \mathrm{Tr}_B\left(\sum_{j\in J,p\in P}C_{jp}(t)\left(\widetilde{A_{jp}}(t)\otimes\widetilde{B_{jp}}(t)\right)\sum_{j'\in J,p'\in P}C_{j'p'}(s)\left(\widetilde{A_{j'p'}}(s)\otimes\widetilde{B_{j'p'}}(s)\right)\widetilde{\rho_S}(t)\rho_B\right. \tag{778}$$

$$-\sum_{j\in J,p\in P}C_{jp}(t)\left(\widetilde{A_{jp}}(t)\otimes\widetilde{B_{jp}}(t)\right)\widetilde{\rho_S}(t)\rho_B\sum_{j'\in J,p'\in P}C_{j'p'}(s)\left(\widetilde{A_{j'p'}}(s)\otimes\widetilde{B_{j'p'}}(s)\right) \tag{779}$$

$$-\sum_{j'\in J,p'\in P}C_{j'p'}(s)\left(\widetilde{A_{j'p'}}(s)\otimes\widetilde{B_{j'p'}}(s)\right)\widetilde{\rho_S}(t)\rho_B\sum_{j\in J,p\in P}C_{jp}(t)\left(\widetilde{A_{jp}}(t)\otimes\widetilde{B_{jp}}(t)\right) \tag{780}$$

$$+\widetilde{\rho_S}(t)\rho_B\sum_{j'\in J,p'\in P}C_{j'p'}(s)\left(\widetilde{A_{j'p'}}(s)\otimes\widetilde{B_{j'p'}}(s)\right)\sum_{j\in J,p\in P}C_{jp}(t)\left(\widetilde{A_{jp}}(t)\otimes\widetilde{B_{jp}}(t)\right)\right)\mathrm{d}s \tag{781}$$

In order to calculate the correlation functions we define:

$$\Lambda_{jpj'p'}(\tau) = \left\langle\widetilde{B_{jp}}(t)\widetilde{B_{j'p'}}(s)\right\rangle_B \tag{782}$$

$$= \left\langle\widetilde{B_{jp}}(\tau)\widetilde{B_{j'p'}}(0)\right\rangle_B \tag{783}$$

Here $s\to t-\tau$ and $\mathrm{Tr}_B\left(\widetilde{B_{jp}}(t)\widetilde{B_{j'p'}}(s)\right) = \left\langle\widetilde{B_{jp}}(t)\widetilde{B_{j'p'}}(s)\right\rangle_B$. To evaluate the trace respect to the bath we need to recall that our master equation depends of elements related to the bath and represented by the operators $\widetilde{B_{jp}}(t)$ and elements related to the system given by $\widetilde{A_{jp}}(t)$. The systems considered are in different Hilbert spaces so $\mathrm{Tr}\left(\widetilde{A_{jp}}(t)\widetilde{B_{j'p'}}(t)\right) = \mathrm{Tr}\left(\widetilde{A_{jp}}(t)\right)\mathrm{Tr}\left(\widetilde{B_{j'p'}}(t)\right)$. The correlation functions relevant of the master equation (781) are:

$$\text{Tr}_B\left(\widetilde{B_{jp}}(t)\,\widetilde{B_{j'p'}}(s)\,\rho_B\right) = \left\langle \widetilde{B_{jp}}(t)\,\widetilde{B_{j'p'}}(s)\right\rangle_B \tag{784}$$

$$= \left\langle \widetilde{B_{jp}}(0)\,\widetilde{B_{j'p'}}(0)\right\rangle_B \tag{785}$$

$$= \Lambda_{jpj'p'}(\tau) \tag{786}$$

$$\text{Tr}_B\left(\widetilde{B_{jp}}(t)\,\rho_B\,\widetilde{B_{j'p'}}(s)\right) = \text{Tr}_B\left(\widetilde{B_{j'p'}}(s)\,\widetilde{B_{jp}}(t)\,\rho_B\right) \tag{787}$$

$$= \left\langle \widetilde{B_{j'p'}}(s)\,\widetilde{B_{jp}}(t)\right\rangle_B \tag{788}$$

$$= \left\langle \widetilde{B_{j'p'}}(-\tau)\,\widetilde{B_{jp}}(0)\right\rangle_B \tag{789}$$

$$= \Lambda_{j'p'jp}(-\tau) \tag{790}$$

$$\text{Tr}_B\left(\widetilde{B_{j'p'}}(s)\,\rho_B\,\widetilde{B_{jp}}(t)\right) = \text{Tr}_B\left(\widetilde{B_{jp}}(t)\,\widetilde{B_{j'p'}}(s)\,\rho_B\right) \tag{791}$$

$$= \left\langle \widetilde{B_{jp}}(t)\,\widetilde{B_{j'p'}}(s)\right\rangle_B \tag{792}$$

$$= \left\langle \widetilde{B_{jp}}(\tau)\,\widetilde{B_{j'p'}}(0)\right\rangle_B \tag{793}$$

$$= \Lambda_{jpj'p'}(\tau) \tag{794}$$

$$\text{Tr}_B\left(\rho_B\,\widetilde{B_{j'p'}}(s)\,\widetilde{B_{jp}}(t)\right) = \text{Tr}_B\left(\widetilde{B_{j'p'}}(s)\,\widetilde{B_{jp}}(t)\,\rho_B\right) \tag{795}$$

$$= \left\langle \widetilde{B_{j'p'}}(s)\,\widetilde{B_{jp}}(t)\right\rangle_B \tag{796}$$

$$= \left\langle \widetilde{B_{j'p'}}(-\tau)\,\widetilde{B_{jp}}(0)\right\rangle_B \tag{797}$$

$$= \Lambda_{j'p'jp}(-\tau) \tag{798}$$

We made use of the cyclic property for the trace to evaluate the correlation functions, from the equations obtained in (774)and (781) and using the equations (784)-(798) we can re-write:

$$\frac{\mathrm{d}\widetilde{\overline{\rho_S}}(t)}{\mathrm{d}t} = -\int_0^t \sum_{j,j',p,p'} \left(C_{jp}(t)\,C_{j'p'}(s)\left(\Lambda_{jpj'p'}(\tau)\,\widetilde{A_{jp}}(t)\,\widetilde{A_{j'p'}}(s)\,\widetilde{\overline{\rho_S}}(t) - \Lambda_{j'p'jp}(-\tau)\,\widetilde{A_{jp}}(t)\,\widetilde{\overline{\rho_S}}(t)\,\widetilde{A_{j'p'}}(s)\right)\right. \tag{799}$$

$$\left. + C_{jp}(t)\,C_{j'p'}(s)\left(\Lambda_{j'p'jp}(-\tau)\,\widetilde{\overline{\rho_S}}(t)\,\widetilde{A_{j'p'}}(s)\,\widetilde{A_{jp}}(t) - \Lambda_{jpj'p'}(\tau)\,\widetilde{A_{j'p'}}(s)\,\widetilde{\overline{\rho_S}}(t)\,\widetilde{A_{jp}}(t)\right)\right)\mathrm{d}s \tag{800}$$

$$= -\int_0^t \sum_{jj'pp'}\left(C_{jp}(t)\,C_{j'p'}(s)\left(\Lambda_{jpj'p'}(\tau)\left[\widetilde{A_{jp}}(t),\widetilde{A_{j'p'}}(s)\,\widetilde{\overline{\rho_S}}(t)\right] + \Lambda_{j'p'jp}(-\tau)\left[\widetilde{\overline{\rho_S}}(t)\,\widetilde{A_{j'p'}}(s),\widetilde{A_{jp}}(t)\right]\right)\right) \tag{801}$$

Rearranging and identofying the commutators allow us to write a more simplified version

$$\frac{\mathrm{d}\,\overline{\rho_S}(t)}{\mathrm{d}t} = -\int_0^t \sum_{jj'pp'}\left(C_{jp}(t)\,C_{j'p'}(t-\tau)\left(\Lambda_{jpj'p'}(\tau)\left[A_{jp}(t),A_{j'p'}(t-\tau,t)\,\overline{\rho_S}(t)\right] + \Lambda_{j'p'jp}(-\tau)\left[\overline{\rho_S}(t)A_{j'p'}(t-\tau,t),A_{jp}(t)\right]\right)\right)\mathrm{d}\tau - \mathrm{i}\left[H_S(t),\overline{\rho_S}(t)\right] \tag{802}$$

For this case we used that $A_{jp}(t-\tau,t) = U(t)\,U^\dagger(t-\tau)\,A_{jp}(t)\,U(t-\tau)\,U^\dagger(t)$. This is a non-Markovian equation.

VIII.   BIBLIOGRAPHY

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