

Dynamical equations of a qubit coupled to a cavity decaying into a bosonic bath – via SPIN-BOSON

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The Hamiltonian is given by :

$$\begin{aligned}\hat{H} = & \sum_{i=0}^{N_q-1} \omega_{\text{qb}}^i |i\rangle \langle i| + \omega_{\text{cav}} \hat{a}^\dagger \hat{a} + \sum_{k=1} \omega_{\text{bath}}^k \hat{d}_k^\dagger \hat{d}_k \\ & + (a + a^\dagger) \sum_{i,j}^{N_q-1} g_{i,j}^{\text{qb-cav}} |i\rangle \langle j| \\ & + a^\dagger \sum_{k=1} \gamma_k d_k + a \sum_{k=1} \gamma_k^* d_k^\dagger \\ & + A_d \cos(\omega^{\text{drive}} t) (a + a^\dagger)\end{aligned}\quad (1)$$

I. DIAGONALISATION OF THE FREE BOSONIC MODES

By combining the field modes together:

$$a_0^\dagger \equiv a^\dagger \quad \text{if} \quad (2)$$

$$a_p^\dagger \equiv d_k^\dagger \quad \text{if} \quad p = k \neq 0, \quad (3)$$

we can obtain:

$$H = \sum_{i=0}^{N_q-1} \omega_{\text{qb}}^i |i\rangle \langle i| + (a_0 + a_0^\dagger) \sum_{i,j}^{N_q-1} g_{i,j}^{\text{qb-cav}} |i\rangle \langle j| + \sum_{p,p'} h_{pp'} a_p^\dagger a_{p'} + A(t) (a_0 + a_0^\dagger), \quad (4)$$

with

$$\begin{aligned}h_{00} &= \omega_{\text{cav}} \\ h_{kk} &= \omega_{\text{bath}}^k \\ h_{0k} &= h_{k0}^* = \gamma_k \\ h_{pp'} &= 0 \quad \text{else.}\end{aligned}\quad (5)$$

Diagonalising the matrix $h_{pp'}$ provides normal modes b_p of the problem:

$$\sum_{pp'} h_{pp'} a_p^\dagger a_{p'} = \sum_p \omega_p b_p^\dagger b_p, \quad (6)$$

In doing so, we have defined the ladder operators in the new basis:

$$b_\sigma = \sum_\mu O_{\sigma\mu}^T a_\mu \quad (7)$$

Conversely,

$$a_0 = \sum_\mu O_{0\mu} b_\mu \quad \text{and} \quad a_k = \sum_\mu O_{k\mu} b_\mu. \quad (8)$$

The matrix O denotes the transfer matrix used to go from the original basis to the new basis. It verifies:

$$D = O^T h O. \quad (9)$$

Hence we obtain the following Hamiltonian:

$$H = \sum_{i=0}^{N_q-1} \omega_{\text{qb}}^i |i\rangle \langle i| + \sum_{i,j}^{N_q-1} \sum_p g_{ij}^p (b_p^\dagger + b_p) |i\rangle \langle j| + \sum_p \omega_p b_p^\dagger b_p + A(t) \sum_p O_{0p} (b_p + b_p^\dagger), \quad (10)$$

where we have defined the coupling $g_{i,i+1}^p$ between the transmon and the normal-mode p as

$$g_{i,j}^p = g_{i,j}^{\text{qb-cav}} O_{0p}. \quad (11)$$

II. GENERAL ALGORITHM

We start with the following wavefunction

$$|\Psi\rangle = \sum_i^{N_q-1} \sum_n^{\text{ncs}} p_{i,n} |i\rangle |z_{i,n}\rangle \quad (12)$$

Here $p_{i,n}$ and $z_{i,n}^p$ are all complex and time dependent variational parameters.

The Lagrangian is given by:

$$\mathcal{L} = \langle \Psi | \frac{i}{2} \overleftrightarrow{\partial}_t - \hat{H} | \Psi \rangle \quad (13)$$

Explicitly:

$$\begin{aligned} \langle \Psi | \vec{\partial}_t | \Psi \rangle &= \left(\sum_m p_m^* \langle z_m | \right) \vec{\partial}_t \left(\sum_n p_n | z_n \rangle \right) \\ &= \sum_{mn} p_m^* \langle z_m | z_n \rangle \left(\dot{p}_n - \frac{1}{2} p_n \left(\sum_p \dot{z}_n^p z_n^{p*} + z_n^p \dot{z}_n^{p*} - 2 z_m^{p*} \dot{z}_n^p \right) \right) \end{aligned} \quad (14)$$

where we have used:

$$\langle z_n | \vec{\partial}_t | z_m \rangle = -\frac{1}{2} \left(\sum_p \dot{z}_m^p z_m^{p*} + z_m^p \dot{z}_m^{p*} - 2 z_n^{p*} \dot{z}_m^p \right) \langle z_n | z_m \rangle$$

Since we have that:

$$\langle \Psi | \overleftarrow{\partial}_t | \Psi \rangle = \langle \Psi | \vec{\partial}_t | \Psi \rangle^*, \quad (15)$$

we obtain:

$$\mathcal{L} = \frac{i}{2} \sum_{mn} \langle z_m | z_n \rangle \left[p_m^* \dot{p}_n - p_n \dot{p}_m^* - \frac{1}{2} p_m^* p_n \left(\sum_p \dot{z}_n^p z_n^{p*} + z_n^p \dot{z}_n^{p*} - 2 z_m^{p*} \dot{z}_n^p - \dot{z}_m^{p*} z_m^p - z_m^{p*} \dot{z}_m^p + 2 z_n^p \dot{z}_m^{p*} \right) \right] - \langle \Psi | \hat{H} | \Psi \rangle \quad (16)$$

The Euler-Lagrange equations are:

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{p}_j^*} - \frac{\partial \mathcal{L}}{\partial p_j^*} = 0 \quad \text{and} \quad \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{z}_j^{p*}} - \frac{\partial \mathcal{L}}{\partial z_j^{p*}} = 0. \quad (17)$$

After p_j^* variation we get

$$\boxed{\sum_m \left(\dot{p}_m - \frac{1}{2} p_m \kappa_{mj} \right) M_{jm} = -i \frac{\partial E}{\partial p_j^*} \equiv P_j} \quad (18)$$

After z_j^{p*} variation we get

$$\sum_m p_m p_j^* \dot{z}_m^p M_{jm} - \frac{1}{4} \sum_m (2\dot{p}_m - p_m \kappa_{mj}) p_j^* (z_j^p - 2z_m^p) M_{jm} + \frac{1}{4} \sum_m (2p_m^* - p_m^* \kappa_{mj}^*) p_j z_j^p M_{mj} = -i \frac{\partial E}{\partial z_j^{p*}} \quad (19)$$

where we have defined:

$$M_{jm} = \langle z_j | z_m \rangle \quad (20)$$

$$\kappa_{mj} = \sum_p \dot{z}_m^p z_m^{p*} + \dot{z}_m^{p*} z_m^p - 2z_j^{p*} \dot{z}_m^p \quad (21)$$

Using (18) to simplify (19), we get:

$$\boxed{\sum_m p_m \dot{z}_m^p M_{jm} + \sum_m (\dot{p}_m - \frac{1}{2} p_m \kappa_{mj}) z_m^p M_{jm} = Z_j^p,} \quad (22)$$

where we have defined:

$$Z_j^p = -i \left[\frac{\partial E}{\partial z_j^{p*}} \frac{1}{p_j^*} + \frac{1}{2} \left(\frac{\partial E}{\partial p_j^*} + \frac{\partial E}{\partial p_j} \frac{p_j}{p_j^*} \right) z_j^p \right] \quad (23)$$

From here on we only derive the equations for \dot{y}_n , as those \dot{z}_n^p can be guessed from the former.

From Eqs. (18) and (22), we get:

$$\begin{aligned} \sum_j M_{nj}^{-1} P_j &= \dot{p}_n - \frac{1}{2} \sum_{mj} p_m \kappa_{mj} M_{nj}^{-1} M_{jm} \\ &= \dot{p}_n - \frac{1}{2} p_n \left(\sum_q \dot{z}_n^q z_n^{q*} + z_n^{q*} \dot{z}_n^q \right) + \sum_{mj} M_{nj}^{-1} M_{jm} p_m \left(\sum_q \dot{z}_j^{q*} z_m^q \right) \end{aligned} \quad (24)$$

$$\sum_j M_{nj}^{-1} Z_j^p = p_n \dot{z}_n^p + \dot{p}_n z_n^p - \frac{1}{2} p_n z_n^p \left(\sum_q \dot{z}_n^q z_n^{q*} + z_n^{q*} \dot{z}_n^q \right) + \sum_{mj} M_{nj}^{-1} M_{jm} p_m z_m^p \left(\sum_q \dot{z}_j^{q*} z_m^q \right) \quad (25)$$

From here we can obtain:

$$\sum_j M_{nj}^{-1} Z_j^p - z_n^p \sum_j M_{nj}^{-1} P_j = p_n \dot{z}_n^p + \sum_{mj} M_{nj}^{-1} M_{jm} p_m \left(\sum_q \dot{z}_j^{q*} z_m^q \right) (z_m^p - z_n^p). \quad (26)$$

Hence:

$$z_i^{p*} \sum_j M_{nj}^{-1} (Z_j^p - z_n^p P_j) = p_n z_i^{p*} \dot{z}_n^p + \sum_{mj} M_{nj}^{-1} M_{jm} p_m \left(\sum_q \dot{z}_j^{q*} z_m^q \right) (z_i^{p*} z_m^p - z_i^{p*} z_n^p). \quad (27)$$

Defining:

$$a_{in} = p_n \left(\sum_p z_i^{p*} \dot{z}_n^p \right), \quad (28)$$

$$b_{in} = \sum_p z_i^{p*} z_n^p, \quad (29)$$

$$A_{in} = \sum_j M_{nj}^{-1} \left(\sum_p z_i^{p*} (Z_j^p - z_n^p P_j) \right), \quad (30)$$

we obtain an equation from Eq. (26) which do not depend on the mode index:

$$\boxed{a_{in} + \sum_{mj} M_{nj}^{-1} M_{jm} a_{jm} (b_{im} - b_{in}) = A_{in}.} \quad (31)$$

In order to solve (31), we define:

$$d_{in} \equiv \sum_l M_{il}^{-1} M_{ln} a_{ln}, \quad (32)$$

and use it to reexpress (31):

$$d_{in} + \sum_m \left(\sum_l M_{il}^{-1} M_{ln} (b_{lm} - b_{ln}) \right) d_{nm} = \sum_l M_{il}^{-1} M_{ln} A_{ln} \quad (33)$$

Hence we get:

$$\boxed{\sum_{mj} (\delta_{mn} \delta_{ij} + \alpha_{inm} \delta_{jn}) d_{jm} = \sum_l M_{il}^{-1} M_{ln} A_{ln}} \quad (34)$$

where:

$$\alpha_{inm} = \sum_l M_{il}^{-1} M_{ln} (b_{lm} - b_{ln}) \quad (35)$$

Once we have solved for d_{in} , we get \dot{z}_n^p and \dot{p}_n from Eqs. (24) and (26):

$$\dot{p}_n = \sum_j M_{nj}^{-1} P_j + \frac{1}{2} p_n \left(\sum_q \dot{z}_n^q \dot{z}_n^{q*} + \dot{z}_n^{q*} \dot{z}_n^q \right) - \sum_m d_{nm} \quad (36)$$

$$\dot{z}_n^p = \frac{1}{p_n} \left(\sum_j M_{nj}^{-1} (Z_j^p - z_n^p P_j) - \sum_m d_{nm} (z_m^p - z_n^p) \right) \quad (37)$$

III. RELEVANT TERM EVALUATIONS

Let us now evaluate the terms on the RHS of the two dynamical equations.

First, the energy is given by:

$$\begin{aligned} E &= \left(\sum_{l,m} p_{l,m}^* \langle l | \langle z_{l,m} | \right) H \left(\sum_{i,n} p_{i,n} | i \rangle | z_{i,n} \rangle \right) \\ E &= \sum_{i,n,m} p_{i,m}^* p_{i,n} \langle z_{i,m} | z_{i,n} \rangle \left[\omega_i^{\text{qb}} + \sum_{p=0} \omega_p z_{i,m}^{p*} z_{i,n}^p + A(t) \sum_p O_{0,p} (z_{i,m}^{p*} + z_{i,n}^p) \right] \\ &\quad + \sum_{i,l,n,m,p} g_{li}^p p_{l,m}^* p_{i,n} \langle z_{l,m} | z_{i,n} \rangle (z_{l,m}^{p*} + z_{i,n}^p) \end{aligned} \quad (38)$$

$$\frac{\partial E}{\partial p_{s,j}^*} = \sum_n p_{s,n} \langle z_{s,j} | z_{s,n} \rangle \left[\omega_s^{\text{qb}} + \sum_p \omega_p z_{s,j}^{p*} z_{s,n}^p + A(t) \sum_p O_{0,p} (z_{s,j}^{p*} + z_{s,n}^p) \right] + \sum_{i,n,p} g_{si}^p p_{i,n} \langle z_{s,j} | z_{i,n} \rangle (z_{s,j}^{p*} + z_{i,n}^p) \quad (39)$$

$$\begin{aligned} \frac{\partial E}{\partial z_{s,j}^{q*}} &= \sum_n p_{s,j}^* p_{s,n} \langle z_{s,j} | z_{s,n} \rangle \left[\omega_q z_{s,n}^q + A(t) O_{0,q} + (z_{s,n}^q - \frac{1}{2} z_{s,j}^q) \left(\omega_s^{\text{qb}} + \sum_{k=0} \omega_k z_{s,j}^{k*} z_{s,n}^k + A(t) \sum_p O_{0,p} (z_{s,j}^{p*} + z_{s,n}^p) \right) \right] \\ &\quad - \frac{1}{2} \sum_n p_{s,n} p_{s,j} \langle z_{s,n} | z_{s,j} \rangle z_{s,j}^q \left[\omega_s^{\text{qb}} + \sum_{p=0} \omega_p z_{s,n}^{p*} z_{s,j}^p + A(t) \sum_p O_{0,p} (z_{s,n}^{p*} + z_{s,j}^p) \right] \\ &\quad + \sum_{in} \left[p_{s,j}^* p_{i,n} \langle z_{s,j} | z_{i,n} \rangle \left(g_{s,i}^q + (z_{i,n}^q - \frac{1}{2} z_{s,j}^q) \sum_p g_{s,i}^p (z_{s,j}^{p*} + z_{i,n}^p) \right) - \frac{1}{2} p_{i,n} p_{s,j} \langle z_{i,n} | z_{s,j} \rangle z_{s,j}^q \sum_p g_{i,s}^p (z_{i,n}^{p*} + z_{s,j}^p) \right] \end{aligned} \quad (40)$$

IV. EVALUATING THE ERROR BETWEEN THE POLARON ANSATZ AND THE EXACT SOLUTION

To check the accuracy of our wave-function, we monitor the norm of the following vector:

$$|\Phi\rangle = \left(i \frac{\vec{\partial}_t}{2} - i \frac{\overleftarrow{\partial}_t}{2} - H \right) |\Psi\rangle \quad (41)$$

$$\langle \Phi | \Phi \rangle = -\frac{1}{2} \Re(\langle \Psi | \vec{\partial}_t \vec{\partial}_t | \Psi \rangle) + \frac{1}{2} \langle \Psi | \overleftarrow{\partial}_t \vec{\partial}_t | \Psi \rangle - 2 \Im(\langle \Psi | \overleftarrow{\partial}_t H | \Psi \rangle) + \langle \Psi | H^2 | \Psi \rangle \quad (42)$$

Noting that:

$$\langle \alpha | \overleftarrow{\partial}_t | \beta \rangle = -\langle \alpha | \beta \rangle \frac{1}{2} \left(\sum_p \dot{\alpha}_p \alpha_p^* + \dot{\alpha}_p^* \alpha_p - 2\beta_p \dot{\alpha}_p^* \right), \quad (43)$$

$$\langle \alpha | \overleftarrow{\partial}_t a_q^\dagger | \beta \rangle = \alpha_q^* \langle \alpha | \overleftarrow{\partial}_t | \beta \rangle + \langle \alpha | \beta \rangle \dot{\alpha}_q^*, \quad (44)$$

$$\langle \alpha | \vec{\partial}_t a_q^\dagger | \beta \rangle = \alpha_q^* \langle \alpha | \vec{\partial}_t | \beta \rangle \quad (45)$$

$$\langle \alpha | a_q \overleftarrow{\partial}_t | \beta \rangle = \beta_q \langle \alpha | \overleftarrow{\partial}_t | \beta \rangle \quad (46)$$

we obtain

$$\begin{aligned} \langle \Psi | \overleftarrow{\partial}_t H | \Psi \rangle &= \sum_{i,n,m} \dot{p}_{i,m}^* p_{i,n} \langle z_{i,m} | z_{i,n} \rangle \left[\omega_i^{\text{qb}} + \sum_{p=0} \omega_p z_{i,m}^{p*} z_{i,n}^p + A(t) \sum_p O_{0p} (z_{im}^{p*} + z_{in}^p) \right] \\ &+ \sum_{i,j,n,m} \dot{p}_{i,m}^* p_{j,n} \langle z_{i,m} | z_{j,n} \rangle \left[\sum_p g_{i,j}^p (z_{i,m}^{p*} + z_{j,n}^p) \right] \\ &+ \sum_{i,n,m} \dot{p}_{i,m}^* p_{i,n} \langle z_{i,m} | z_{i,n} \rangle \left[-\frac{1}{2} \left(\sum_p \dot{z}_{i,m}^p z_{i,m}^{p*} + \dot{z}_{i,m}^{p*} z_{i,m}^p - 2\dot{z}_{i,m}^{p*} z_{i,n}^p \right) \left(\omega_i^{\text{qb}} + \sum_p \omega_p z_{i,m}^{p*} z_{in}^p + A(t) \sum_p O_{0p} (z_{im}^{p*} + z_{in}^p) \right) \right. \\ &\quad \left. + \left(\sum_p \omega_p \dot{z}_{im}^{p*} z_{in}^p + A(t) \sum_p O_{0p} \dot{z}_{im}^{p*} \right) \right] \\ &+ \sum_{i,j,n,m} \dot{p}_{i,m}^* p_{j,n} \langle z_{i,m} | z_{j,n} \rangle \left[-\frac{1}{2} \left(\sum_p \dot{z}_{i,m}^p z_{i,m}^{p*} + \dot{z}_{i,m}^{p*} z_{i,m}^p - 2\dot{z}_{i,m}^{p*} z_{j,n}^p \right) \left(\sum_p g_{i,j}^p (z_{i,m}^{p*} + z_{j,n}^p) \right) + \left(\sum_p g_{ij}^p \dot{z}_{i,m}^{p*} \right) \right] \end{aligned} \quad (47)$$

$$\begin{aligned} \langle \Psi | H^2 | \Psi \rangle &= \sum_{im} \dot{p}_{i,m}^* p_{i,n} \langle z_{i,m} | z_{i,n} \rangle \left[\left(\omega_{\text{qb}}^i + \sum_p \omega_p z_{im}^{p*} z_{in}^p + A(t) \sum_p O_{0p} (z_{im}^{p*} + z_{in}^p) \right)^2 \right. \\ &\quad \left. + \sum_p \omega_p^2 z_{im}^{p*} z_{in}^p + \sum_p \omega_p A(t) O_{0p} (z_{im}^{p*} + z_{in}^p) + A^2(t) \sum_p O_{0p}^2 \right] \\ &+ \sum_{i,j,n,m} \dot{p}_{i,m}^* p_{j,n} \langle z_{i,m} | z_{j,n} \rangle \left[\sum_{pq} \left(\sum_s g_{s,j}^p g_{s,i}^q + 2A(t) O_{0p} g_{ij}^q \right) \left(z_{i,m}^{p*} + z_{j,n}^p \right) \left(z_{i,m}^{q*} + z_{j,n}^q \right) + \sum_p \left(\sum_s g_{s,j}^p g_{s,i}^p + 2A(t) O_{0p} g_{ij}^p \right) \right. \\ &\quad \left. + \left(\omega_{\text{qb}}^i + \omega_{\text{qb}}^j \right) \left(\sum_p g_{ij}^p (z_{im}^{p*} + z_{jn}^p) \right) + 2 \sum_{pq} g_{ji}^q \omega_p z_{jn}^p z_{im}^{p*} \left(z_{jn}^q + z_{im}^{q*} \right) + \sum_p g_{ij}^p \omega_p (z_{jn}^p + z_{im}^{p*}) \right] \end{aligned}$$

$$\begin{aligned} \langle \Psi | \overleftarrow{\partial}_t \vec{\partial}_t | \Psi \rangle &= \sum_i \sum_{m,n} \langle z_{i,m} | z_{i,n} \rangle \left[\dot{p}_{i,m}^* \dot{p}_{i,n} - \frac{1}{2} \dot{p}_{i,m}^* p_{i,n} \sum_p (\dot{z}_{i,n}^p z_{i,n}^{p*} + \dot{z}_{i,n}^{p*} z_{i,n}^p - 2\dot{z}_{i,n}^{p*} z_{i,m}^p) - \frac{1}{2} \dot{p}_{i,m}^* \dot{p}_{i,n} \sum_p (\dot{z}_{i,m}^p z_{i,m}^{p*} + \dot{z}_{i,m}^{p*} z_{i,m}^p - 2\dot{z}_{i,m}^{p*} z_{i,n}^p) \right. \\ &\quad \left. + \dot{p}_{i,m}^* p_{i,n} \left[\sum_p \dot{z}_{i,m}^{p*} z_{i,n}^p + \frac{1}{4} \sum_{p,q} (\dot{z}_{i,m}^p z_{i,m}^{p*} + \dot{z}_{i,m}^{p*} z_{i,m}^p - 2\dot{z}_{i,m}^{p*} z_{i,n}^p) (\dot{z}_{i,n}^q z_{i,n}^{q*} + \dot{z}_{i,n}^{q*} z_{i,n}^q - 2\dot{z}_{i,n}^{q*} z_{i,m}^q) \right] \right] \end{aligned}$$

$$\begin{aligned}
\langle \Psi | \vec{\partial}_t \vec{\partial}_t | \Psi \rangle &= \sum_i \sum_{m,n} p_{i,m}^* \langle z_{i,m} | \vec{\partial}_t \left[\dot{p}_{i,n} |z_{i,n}\rangle + p_{i,n} \vec{\partial}_t |z_{i,n}\rangle \right] = \sum_i \sum_{m,n} p_{i,m}^* \langle z_{i,m} | \left[\ddot{p}_{i,n} |z_{i,n}\rangle + 2\dot{p}_{i,n} \vec{\partial}_t |z_{i,n}\rangle + p_{i,n} \vec{\partial}_t^2 |z_{i,n}\rangle \right] \\
&= \sum_i \sum_{m,n} p_{i,m}^* \left[\ddot{p}_{i,n} \langle z_{i,m} | z_{i,n} \rangle + 2\dot{p}_{i,n} \langle z_{i,m} | \vec{\partial}_t | z_{i,n} \rangle + p_{i,n} \langle z_{i,m} | \vec{\partial}_t^2 | z_{i,n} \rangle \right] \\
&= \sum_i \sum_{m,n} p_{i,m}^* \langle z_{i,m} | z_{i,n} \rangle \left[\ddot{p}_{i,n} - \dot{p}_{i,n} \left(\sum_p \dot{z}_{i,n}^{p*} \dot{z}_{i,n}^p + \dot{z}_{i,n}^p \dot{z}_{i,n}^{p*} - 2\dot{z}_{i,n}^p \dot{z}_{i,n}^{p*} \right) \right. \\
&\quad \left. + p_{i,n} \left(\left(\sum_p \dot{z}_{i,m}^{p*} \dot{z}_{i,n}^p - \frac{1}{2} (\dot{z}_{i,n}^{p*} \dot{z}_{i,n}^p + \dot{z}_{i,n}^p \dot{z}_{i,n}^{p*} + 2\dot{z}_{i,n}^{p*} \dot{z}_{i,n}^p) \right) + \frac{1}{4} \left(\sum_p \dot{z}_{i,n}^p \dot{z}_{i,n}^{p*} + \dot{z}_{i,n}^{p*} \dot{z}_{i,n}^p - 2\dot{z}_{i,n}^p \dot{z}_{i,n}^{p*} \right)^2 \right) \right]
\end{aligned}$$