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

Nicolas Gheeraert

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The Hamiltonian is given by :

$$\hat{H} = 4E_c n^2 - E_J\cos(\varphi) + \omega_c a^\dagger a + ign_0(a^\dagger - a) + \sum_{k=0}^{N}\omega_k a_k^\dagger a_k + i^2\sum_{k=0}^{N} g_k(a^\dagger - a)(a_k^\dagger - a_k) + A(t)(a^\dagger - a)$$
$$\hat{H} = \hat{H}_0 - E_J\cos(\varphi) - \frac{E_J}{2}\varphi^2 + A(t)(a^\dagger - a) \tag{1}$$

To maintain a concise notation we define the operators a_μ, with μ indexing all degrees of freedom of the system (qubit [$\mu = 0$], cavity [$\mu = 1$], N modes [$\mu = 2..N+2$]):

$$a_0 = \frac{1}{\sqrt{2}}\left(\left(\frac{E_J}{8E_C}\right)^{1/4}\varphi_0 + i\left(\frac{8E_C}{E_J}\right)^{1/4} n_0\right)$$
$$a_\mu = \frac{1}{\sqrt{2}}\left(\sqrt{\omega_\mu}\varphi_\mu + i\frac{1}{\sqrt{\omega_\mu}}n_\mu\right) \quad \text{for} \quad [\mu \neq 0]. \tag{2}$$

Equivalently,

$$\varphi_0 = \frac{1}{\sqrt{2}}\left(\frac{8E_C}{E_J}\right)^{1/4}(a_0^\dagger + a_0) \qquad \varphi_\mu = \frac{1}{\sqrt{2\omega_\mu}}(a_\mu^\dagger + a_\mu)$$
$$n_0 = \frac{i}{\sqrt{2}}\left(\frac{E_J}{8E_C}\right)^{1/4}(a_0^\dagger - a_0) \qquad n_\mu = i\frac{\sqrt{\omega_\mu}}{\sqrt{2}}(a_\mu^\dagger - a_\mu) \tag{3}$$

I. DIAGONALISATION OF THE FREE BOSONIC MODES

The linearised Hamiltonian H_0 is given by:

$$H_0 = 4E_c n_0^2 + \frac{E_J}{2}\varphi_0^2 + \omega_1 a_1^\dagger a_1 + ign_0(a_1^\dagger - a_1) + \sum_{\mu=2}^{N+2}\omega_\mu a_\mu^\dagger a_\mu + i^2\sum_{\mu=2}^{N+2} g_\mu(a_1^\dagger - a_1)(a_\mu^\dagger - a_\mu) + A(t)(a_1^\dagger - a_1) \tag{4}$$

It can be put in a simple form by successively rescaling the phase and charge number operators, i.e.

$$\varphi_\mu \to \bar{\varphi}_\mu/\eta_\mu \qquad n_\mu \to \eta_\mu \bar{n}_\mu, \tag{5}$$

with $\eta_0 = \sqrt{E_J}$, and $\eta_\mu = \omega_\mu$ for $\mu \neq 0$, and then diagonalising the Hamiltonian:

$$H_0 = \frac{1}{2}\sum_\mu \bar{\varphi}_\mu\bar{\varphi}_\mu + \frac{1}{2}\sum_{\sigma\mu}\bar{n}_\sigma M_{\sigma\mu}\bar{n}_\mu$$
$$= \frac{1}{2}\sum_\mu \bar{\varphi}'_\mu\bar{\varphi}'_\mu + \frac{1}{2}\sum_\mu \Omega_\mu^2\bar{n}'_\mu\bar{n}'_\mu$$
$$= \sum_\mu \Omega_\mu b_\mu^\dagger b_\mu. \tag{6}$$

In doing so, we have defined the phase and charge number operators in the new basis:

$$\bar{n}'_\sigma = \sum_\mu O^T_{\sigma\mu}\bar{n}_\mu \quad \text{and} \quad \bar{\varphi}'_\sigma = \sum_\mu O^T_{\sigma\mu}\bar{\varphi}_\mu. \tag{7}$$

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

$$D = O^T M O. \tag{8}$$

In this new basis the ladder operators are given by:

$$b_\mu = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{\Omega_\mu}}\bar{\varphi}'_\mu + i\sqrt{\Omega_\mu}\bar{n}'_\mu\right). \tag{9}$$

We now need to express the original ladder operators in the terms of the operators in the new basis. We start by expressing the original phase and charge number operators in terms of b_μ and $b_\mu^\dagger$:

$$\begin{aligned}
\varphi_\sigma &= \frac{\bar{\varphi}_\sigma}{\eta_\sigma} = \frac{1}{\eta_\sigma}\sum_\mu O_{\sigma\mu}\bar{\varphi}'_\mu = \frac{1}{\eta_\sigma}\sum_\mu \frac{O_{\sigma\mu}\sqrt{\Omega_\mu}}{\sqrt{2}}(b_\mu^\dagger + b_\mu)\\
n_\sigma &= \eta_\sigma \bar{n}_\sigma = \eta_\sigma \sum_\mu O_{\sigma\mu}\bar{n}'_\mu = i\eta_\sigma \sum_\mu \frac{O_{\sigma\mu}}{\sqrt{2\Omega_\mu}}(b_\mu^\dagger - b_\mu)
\end{aligned} \tag{10}$$

Hence:

$$\begin{aligned}
a_0^\dagger + a_0 &= \left(\frac{E_J}{8E_C}\right)^{1/4}\sum_\mu \frac{O_{0\mu}\sqrt{\Omega_\mu}}{\eta_0}(b_\mu^\dagger + b_\mu) = \sum_\mu T_{0\mu}(b_\mu^\dagger + b_\mu)\\
a_0^\dagger - a_0 &= \left(\frac{8E_C}{E_J}\right)^{1/4}\sum_\mu \frac{\eta_0 O_{0\mu}}{\sqrt{\Omega_\mu}}(b_\mu^\dagger - b_\mu) = \sum_\mu V_{0\mu}(b_\mu^\dagger - b_\mu).\\
a_\sigma^\dagger + a_\sigma &= \sum_\mu \frac{O_{\sigma\mu}\sqrt{\omega_\sigma\Omega_\mu}}{\eta_\sigma}(b_\mu^\dagger + b_\mu) = \sum_\mu T_{\sigma\mu}(b_\mu^\dagger + b_\mu)\\
a_\sigma^\dagger - a_\sigma &= \sum_\mu \frac{\eta_\sigma O_{\sigma\mu}}{\sqrt{\omega_\sigma\Omega_\mu}}(b_\mu^\dagger - b_\mu) = \sum_\mu V_{\sigma\mu}(b_\mu^\dagger - b_\mu).
\end{aligned} \tag{11}$$

Finally, we obtain:

$$\boxed{\begin{aligned}
a_\sigma^\dagger &= \frac{1}{2}\sum_\mu \Big[T_{\sigma\mu} + V_{\sigma\mu}\Big]b_\mu^\dagger + \frac{1}{2}\sum_\mu \Big[T_{\sigma\mu} - V_{\sigma\mu}\Big]b_\mu\\
a_\sigma &= \frac{1}{2}\sum_\mu \Big[T_{\sigma\mu} - V_{\sigma\mu}\Big]b_\mu^\dagger + \frac{1}{2}\sum_\mu \Big[T_{\sigma\mu} + V_{\sigma\mu}\Big]b_\mu
\end{aligned}} \tag{12}$$

After diagonalising the linear part we get:

$$\begin{aligned}
H &= \sum_\mu \Omega_\mu b_\mu^\dagger b_\mu - E_J\cos(\varphi_0) - \frac{E_J}{2}\varphi_0^2 + A(t)(a_1^\dagger - a_1)\\
&= \sum_\mu \Omega_\mu b_\mu^\dagger b_\mu - E_J\cos\left(\sum_\mu u_\mu(b_\mu^\dagger + b_\mu)\right) - \frac{E_J}{2}\left[\sum_\mu u_\mu(b_\mu^\dagger + b_\mu)\right]^2 + A(t)\sum_\mu V_{1\mu}(b_\mu^\dagger - b_\mu)
\end{aligned} \tag{13}$$

with $u_\mu = \sqrt{\frac{\Omega_\mu}{2E_J}}O_{0\mu}$.

II. GENERAL ALGORITHM

We start with the following wavefunction

$$|\Psi\rangle = \sum_n^{\mathrm{ncs}} p_n\,|z_n\rangle \tag{14}$$

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

The Lagrangian is given by:

$$\begin{aligned}\mathscr{L} &= \langle\Psi|\frac{i}{2}\overleftrightarrow{\partial_t} - \hat{H}|\Psi\rangle \\ &= \langle\Psi|\frac{i}{2}\overrightarrow{\partial_t} - \frac{i}{2}\overleftarrow{\partial_t} - \hat{H}|\Psi\rangle \end{aligned} \tag{15}$$

Explicitely:

$$\begin{aligned}\langle\Psi|\overrightarrow{\partial}_t|\Psi\rangle &= \left(\sum_m p^\star_m \langle z_m|\right)\overrightarrow{\partial}_t\left(\sum_n p_n|z_n\rangle\right) \\ &= \sum_{mn} p^\star_m \langle z_m|z_n\rangle \left(\dot{p}_n - \frac{1}{2}p_n\left(\sum_p \dot{z}^p_n z^{p\star}_n + z^p_n \dot{z}^{p\star}_n - 2z^{p\star}_m \dot{z}^p_n\right)\right)\end{aligned} \tag{16}$$

where we have used:

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

Moreover, since we have that:

$$\langle\Psi|\overleftarrow{\partial_t}|\Psi\rangle = \langle\Psi|\overrightarrow{\partial_t}|\Psi\rangle^\star, \tag{17}$$

we obtain:

$$\mathscr{L} = \frac{i}{2}\sum_{mn}\langle z_m|z_n\rangle\left[p^\star_m \dot{p}_n - p_n \dot{p}^\star_m - \frac{1}{2}p^\star_m p_n\left(\sum_p \dot{z}^p_n z^{p\star}_n + z^p_n \dot{z}^{p\star}_n - 2z^{p\star}_m \dot{z}^p_n - \dot{z}^{p\star}_m z^p_m - z^{p\star}_m \dot{z}^p_m + 2z^p_n \dot{z}^{p\star}_m\right)\right] - \langle\Psi|H|\Psi\rangle \tag{18}$$

The Euler-Lagrange equations are:

$$\frac{d}{dt}\frac{\partial\mathscr{L}}{\partial\dot{p}^\star_j} - \frac{\partial\mathscr{L}}{\partial p^\star_j} = 0 \quad \text{and} \qquad \frac{d}{dt}\frac{\partial\mathscr{L}}{\partial\dot{z}^{p\star}_j} - \frac{\partial\mathscr{L}}{\partial z^{p\star}_j} = 0. \tag{19}$$

After $p^\star_j$ variation we get

$$\boxed{\sum_m\left(\dot{p}_m - \frac{1}{2}p_m\boldsymbol{\kappa}_{mj}\right)M_{jm} = -i\frac{\partial E}{\partial p^\star_j} \equiv P_j} \tag{20}$$

After $z^{p\star}_j$ variation we get

$$\sum_m p_m p^\star_j \dot{z}^p_m M_{jm} - \frac{1}{4}\sum_m\left(2\dot{p}_m - p_m\boldsymbol{\kappa}_{mj}\right)p^\star_j(z^p_j - 2z^p_m)M_{jm} + \frac{1}{4}\sum_m\left(2\dot{p}^\star_m - p^\star_m\boldsymbol{\kappa}^\star_{mj}\right)p_j z^p_j M_{mj} = -i\frac{\partial E}{\partial z^{p\star}_j} \tag{21}$$

where we have defined:

$$M_{jm} = \langle z_j|z_m\rangle \tag{22}$$

$$\kappa_{mj} = \sum_p \dot{z}^p_m z^{p\star}_m + \dot{z}^{p\star}_m z^p_m - 2z^{p\star}_j \dot{z}^p_m \tag{23}$$

Using (20) to simplify (21), we get:

$$\boxed{\sum_m p_m \dot{z}_m^p M_{jm} + \sum_m (\dot{p}_m - \frac{1}{2} p_m \kappa_{mj}) z_m^p M_{jm} = Z_j^p,} \tag{24}$$

where we have defined:

$$Z_j^p = -i \left[\frac{\partial E}{\partial z_j^{p\star}} \frac{1}{p_j^\star} + \frac{1}{2} \left(\frac{\partial E}{\partial p_j^\star} + \frac{\partial E}{\partial p_j} \frac{p_j}{p_j^\star} \right) z_j^p \right] \tag{25}$$

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. (20) and (24), we get:

$$\sum_j M_{nj}^{-1} P_j = \dot{p}_n - \frac{1}{2} \sum_{mj} p_m \kappa_{mj} M_{nj}^{-1} M_{jm}$$
$$= \dot{p}_n - \frac{1}{2} p_n \Big(\sum_q \dot{z}_n^q z_n^{q\star} + \dot{z}_n^{q\star} z_n^q \Big) + \sum_{mj} M_{nj}^{-1} M_{jm} p_m \Big(\sum_q z_j^{q\star} \dot{z}_m^q \Big) \tag{26}$$

$$\sum_j M_{nj}^{-1} Z_j^p = p_n \dot{z}_n^p + \dot{p}_n z_n^p - \frac{1}{2} p_n z_n^p \Big(\sum_q \dot{z}_n^q z_n^{q\star} + \dot{z}_n^{q\star} z_n^q \Big) + \sum_{mj} M_{nj}^{-1} M_{jm} p_m z_m^p \Big(\sum_q z_j^{q\star} \dot{z}_m^q \Big) \tag{27}$$

From here we can obtain:

$$\sum_j M_{nj}^{-1} Z_j^p - z_n^p \sum_j M_{nj}^{-1} P_j = p_n \dot{z}_n^p + \sum_{mj} M_{nj}^{-1} M_{jm} p_m \Big(\sum_q z_j^{q\star} \dot{z}_m^q \Big) (z_m^p - z_n^p). \tag{28}$$

Hence:

$$z_i^{p\star} \sum_j M_{nj}^{-1} \Big(Z_j^p - z_n^p P_j \Big) = p_n z_i^{p\star} \dot{z}_n^p + \sum_{mj} M_{nj}^{-1} M_{jm} p_m \Big(\sum_q z_j^{q\star} \dot{z}_m^q \Big) (z_i^{p\star} z_m^p - z_i^{p\star} z_n^p). \tag{29}$$

Defining:

$$a_{in} = p_n \Big(\sum_p z_i^{p\star} \dot{z}_n^p \Big), \tag{30}$$

$$b_{in} = \sum_p z_i^{p\star} z_n^p, \tag{31}$$

$$A_{in} = \sum_j M_{nj}^{-1} \Big(\sum_p z_i^{p\star} (Z_j^p - z_n^p P_j) \Big), \tag{32}$$

we obtain an equation from Eq. (28) which do not depend on the mode index:

$$\boxed{a_{in} + \sum_{mj} M_{nj}^{-1} M_{jm} a_{jm} (b_{im} - b_{in}) = A_{in}.} \tag{33}$$

In order to solve (33), we define:

$$d_{in} \equiv \sum_l M_{il}^{-1} M_{ln} a_{ln}, \tag{34}$$

and use it to reexpress (33):

$$d_{in} + \sum_m \left(\sum_l M_{il}^{-1} M_{ln} (b_{lm} - b_{ln}) \right) d_{nm} = \sum_l M_{il}^{-1} M_{ln} A_{ln} \tag{35}$$

Hence we get:

$$\boxed{\sum_{mj} (\delta_{mn} \delta_{ij} + \alpha_{inm} \delta_{jn}) d_{jm} = \sum_l M_{il}^{-1} M_{ln} A_{ln}} \tag{36}$$

where:

$$\alpha_{inm} = \sum_l M_{il}^{-1} M_{ln}(b_{lm} - b_{ln}) \tag{37}$$

Once we have solved for d_{in}, we get $\dot{z}_n^p$ and $\dot{p}_n$ from Eqs. (26) and (28):

$$\boxed{\begin{aligned} \dot{p}_n &= \sum_j M_{nj}^{-1} P_j + \frac{1}{2} p_n \Big(\sum_q \dot{z}_n^q z_n^{q\star} + \dot{z}_n^{q\star} z_n^q \Big) - \sum_m d_{nm} && (38) \\ \dot{z}_n^p &= \frac{1}{p_n} \left(\sum_j M_{nj}^{-1} (Z_j^p - z_n^p P_j) - \sum_m d_{nm} (z_m^p - z_n^p) \right) && (39) \end{aligned}}$$

III. RELEVANT TERM EVALUATIONS

Let us now evaluate the terms on the RHS dynamical equations (20) and (24).

First let us note:

$$\begin{aligned} \langle z^m | \Big(\sum_\mu u_\mu (b_\mu^\dagger + b_\mu) \Big)^2 | z^n \rangle &= \langle z^m | z^n \rangle \left[\Big(\sum_\mu u_\mu (z_\mu^{m\star} + z_\mu^n) \Big)^2 + \sum_\mu u_\mu^2 \right] \\ \langle z^m | \cos \left(\sum_\mu u_\mu (b_\mu^\dagger + b_\mu) \right) | z^n \rangle &= \langle z^m | z^n \rangle \cos \left[\sum_\mu u_\mu (z_\mu^{m\star} + z_\mu^n) \right] e^{-\frac{1}{2} \sum_\mu u_\mu^2} \end{aligned} \tag{40}$$

First, the energy is given by:

$$\begin{aligned} E &= \Big(\sum_m p_m^\star \langle z^m | \Big) \left[\sum_\mu \Omega_\mu b_\mu^\dagger b_\mu - E_J \cos \left(\sum_\mu u_\mu (b_\mu^\dagger + b_\mu) \right) - \frac{E_J}{2} \left[\sum_\mu u_\mu (b_\mu^\dagger + b_\mu) \right]^2 + A(t) \sum_\mu V_{1\mu} (b_\mu^\dagger - b_\mu) \right] \Big(\sum_n p_n | z^n \rangle \Big) \\ &= \sum_{mn} p_m^\star p_n \langle z^m | z^n \rangle \left[\sum_\mu \Omega_\mu z_\mu^{m\star} z_\mu^n - E_J \cos \left[\sum_\mu u_\mu (z_\mu^{m\star} + z_\mu^n) \right] e^{-\frac{1}{2} \sum_\mu u_\mu^2} - \frac{E_J}{2} \left(\Big(\sum_\mu u_\mu (z_\mu^{m\star} + z_\mu^n) \Big)^2 + \sum_\mu u_\mu^2 \right) + A(t) \sum_\mu V_{1\mu} (z_\mu^{m\star} - z_\mu^n) \right] \end{aligned} \tag{41}$$

From this expression we can calculate the derivatives with respect to $p^{j\star}$ and $z_\sigma^{j\star}$:

$$\begin{aligned} \frac{\partial E}{\partial p^{j\star}} &= \sum_n p_n \langle z^j | z^n \rangle \left[\sum_\mu \Omega_\mu z_\mu^{j\star} z_\mu^n - E_J \cos \left[\sum_\mu u_\mu (z_\mu^{j\star} + z_\mu^n) \right] e^{-\frac{1}{2} \sum_\mu u_\mu^2} - \frac{E_J}{2} \left(\Big(\sum_\mu u_\mu (z_\mu^{j\star} + z_\mu^n) \Big)^2 + \sum_\mu u_\mu^2 \right) + A(t) \sum_\mu V_{1\mu} (z_\mu^{j\star} - z_\mu^n) \right] \\ \frac{\partial E}{\partial z_\sigma^{j\star}} &= \sum_n p_j^\star p_n \langle z^j | z^n \rangle \left[-\frac{1}{2} (z_\sigma^j - 2 z_\sigma^n) \left(\sum_\mu \Omega_\mu z_\mu^{j\star} z_\mu^n - E_J \cos \left[\sum_\mu u_\mu (z_\mu^{j\star} + z_\mu^n) \right] e^{-\frac{1}{2} \sum_\mu u_\mu^2} - \frac{E_J}{2} \left(\Big(\sum_\mu u_\mu (z_\mu^{j\star} + z_\mu^n) \Big)^2 + \sum_\mu u_\mu^2 \right) \right. \right. \\ &\qquad \left. \left. + A(t) \sum_\mu V_{1\mu} (z_\mu^{j\star} - z_\mu^n) \right) + A(t) V_{1\sigma} + z_\sigma^n \Omega_\sigma - u_\sigma E_J \left(- e^{-\frac{1}{2} \sum_\mu u_\mu^2} \sin \Big(\sum_\mu u_\mu (z_\mu^{j\star} + z_\mu^n) \Big) + \sum_\mu u_\mu (z_\mu^{j\star} + z_\mu^n) \right) \right] \\ &\quad - \frac{1}{2} \sum_m p_m^\star p_j z_\sigma^j \langle z^m | z^j \rangle \left[\sum_\mu \Omega_\mu z_\mu^{m\star} z_\mu^j - E_J \cos \left[\sum_\mu u_\mu (z_\mu^{m\star} + z_\mu^j) \right] e^{-\frac{1}{2} \sum_\mu u_\mu^2} - \frac{E_J}{2} \left(\Big(\sum_\mu u_\mu (z_\mu^{m\star} + z_\mu^j) \Big)^2 + \sum_\mu u_\mu^2 \right) \right. \\ &\qquad \left. + A(t) \left(\sum_\mu V_{1\mu} (z_\mu^{m\star} - z_\mu^j) \right) \right] \end{aligned} \tag{42}$$

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:

$$|\Phi\rangle = \left(i\frac{\overrightarrow{\partial_t}}{2} - i\frac{\overleftarrow{\partial_t}}{2} - H \right) |\Psi\rangle \tag{43}$$

$$\boxed{\langle\Phi|\Phi\rangle = -\frac{1}{2}\Re\big(\langle\Psi|\ \overrightarrow{\partial_t}\ \overrightarrow{\partial_t}\ |\Psi\rangle\big) + \frac{1}{2}\ \langle\Psi|\ \overleftarrow{\partial_t}\ \overrightarrow{\partial_t}\ |\Psi\rangle + 2\ i\ \Re\big(\langle\Psi|\ \overleftarrow{\partial_t}\ H\ |\Psi\rangle\big) + \langle\Psi|H^2|\Psi\rangle} \tag{44}$$