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 :

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

I. DIAGONALISATION OF THE FREE BOSONIC MODES

By combining the field modes together:

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

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

we can obtain:

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

with

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

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

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

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

$$b_\sigma = \sum_\mu O_{\sigma\mu}^T a_\mu \tag{7}$$

Conversely,

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

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

$$D = O^T h O. \tag{9}$$

Hence we obtain the following Hamiltonian:

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

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

$$g_{i,j}^{p}=g_{i,j}^{\mathrm{qb-cav}}O_{0p}.\tag{11}$$

II. GENERAL ALGORITHM

We start with the following wavefunction

$$\left|\Psi\right\rangle=\sum_{i}^{N_q-1}\sum_{n}^{\mathrm{ncs}}p_{i,n}\left|i\right\rangle\left|z_{i,n}\right\rangle\tag{12}$$

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

The Lagrangian is given by:

$$\mathscr{L}=\langle\Psi|\frac{i}{2}\overleftrightarrow{\partial_t}-\hat{H}|\Psi\rangle\tag{13}$$

Explicitely:

$$\begin{aligned}\langle\Psi|\overrightarrow{\partial}_t|\Psi\rangle&=\left(\sum_{m}p_m^{\star}\left\langle z_m\right|\right)\overrightarrow{\partial}_t\left(\sum_{n}p_n\left|z_n\right\rangle\right)\\&=\sum_{mn}p_m^{\star}\left\langle z_m|z_n\right\rangle\left(\dot{p}_n-\frac{1}{2}p_n\Big(\sum_{p}\dot{z}_n^{p}z_n^{p\star}+z_n^{p}\dot{z}_n^{p\star}-2z_m^{p\star}\dot{z}_n^{p}\Big)\right)\end{aligned}\tag{14}$$

where we have used:

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

Since we have that:

$$\langle\Psi|\overleftarrow{\partial_t}|\Psi\rangle=\langle\Psi|\overrightarrow{\partial_t}|\Psi\rangle^{\star},\tag{15}$$

we obtain:

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

The Euler-Lagrange equations are:

$$\frac{d}{dt}\frac{\partial\mathscr{L}}{\partial\dot{p}_j^{\star}}-\frac{\partial\mathscr{L}}{\partial p_j^{\star}}=0\quad\text{and}\qquad\frac{d}{dt}\frac{\partial\mathscr{L}}{\partial\dot{z}_j^{p\star}}-\frac{\partial\mathscr{L}}{\partial z_j^{p\star}}=0.\tag{17}$$

After $p_j^{\star}$ variation we get

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

After $z_j^{p\star}$ variation we get

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

where we have defined:

$$M_{jm} = \langle z_j | z_m \rangle \tag{20}$$
$$\kappa_{mj} = \sum_p \dot{z}_m^p z_m^{p\star} + \dot{z}_m^{p\star} z_m^p - 2z_j^{p\star}\dot{z}_m^p \tag{21}$$

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

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

where we have defined:

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

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:

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

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

From here we can obtain:

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

Hence:

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

Defining:

$$a_{in} = p_n\left(\sum_p z_i^{p\star}\dot{z}_n^p\right), \tag{28}$$
$$b_{in} = \sum_p z_i^{p\star} z_n^p, \tag{29}$$
$$A_{in} = \sum_j M_{nj}^{-1}\left(\sum_p z_i^{p\star}(Z_j^p - z_n^p P_j)\right), \tag{30}$$

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

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

In order to solve (31), we define:

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

and use it to reexpress (31):

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

Hence we get:

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

where:

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

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

$$\dot{p}_n = \sum_j M_{nj}^{-1} P_j + \frac{1}{2} p_n \Big(\sum_q \dot{z}_n^q z_n^{q\star} + \dot{z}_n^{q\star} z_n^q \Big) - \sum_m d_{nm} \tag{36}$$

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

III. RELEVANT TERM EVALUATIONS

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

First, the energy is given by:

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

$$\frac{\partial E}{\partial p_{s,j}^\star} = \sum_n p_{s,n} \langle z_{s,j}|z_{s,n}\rangle \Big[\omega_s^{\mathrm{qb}} + \sum_p \omega_p z_{s,j}^{p\star} z_{s,n}^p + A(t) \sum_p O_{0,p} \big(z_{s,j}^{p\star} + z_{s,n}^p \big) \Big] + \sum_{i,n,p} g_{si}^p p_{i,n} \langle z_{s,j}|z_{i,n}\rangle \big(z_{s,j}^{p\star} + z_{i,n}^p \big) \tag{39}$$

$$\begin{aligned}
\frac{\partial E}{\partial z_{s,j}^{q\star}} =& \sum_n p_{s,j}^\star p_{s,n} \langle z_{s,j}|z_{s,n}\rangle \Big[\omega_q z_{s,n}^q + A(t) O_{0,q} + (z_{s,n}^q - \tfrac{1}{2} z_{s,j}^q) \Big(\omega_s^{\mathrm{qb}} + \sum_{k=0} \omega_p z_{s,j}^{p\star} z_{s,n}^p + A(t) \sum_p O_{0,p} \big(z_{s,j}^{p\star} + z_{s,n}^p \big) \Big) \Big] \\
&- \frac{1}{2} \sum_n p_{s,n}^\star p_{s,j} \langle z_{s,n}|z_{s,j}\rangle z_{s,j}^q \Big[\omega_{\mathrm{s}}^{\mathrm{qb}} + \sum_{p=0} \omega_p z_{s,n}^{p\star} z_{s,j}^p + A(t) \sum_p O_{0,p} \big(z_{s,n}^{p\star} + z_{s,j}^p \big) \Big] \\
&+ \sum_{in} \Big[p_{s,j}^\star p_{i,n} \langle z_{s,j}|z_{i,n}\rangle \Big(g_{s,i}^q + (z_{i,n}^q - \tfrac{1}{2} z_{s,j}^q) \sum_p g_{s,i}^p (z_{s,j}^{p\star} + z_{i,n}^p) \Big) - \frac{1}{2} p_{i,n}^\star p_{s,j} \langle z_{i,n}|z_{s,j}\rangle z_{s,j}^q \sum_p g_{i,s}^p (z_{i,n}^{p\star} + z_{s,j}^p) \Big]
\end{aligned} \tag{40}$$

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:

$$|\Phi\rangle = \left(i\frac{\overrightarrow{\partial_t}}{2} - i\frac{\overleftarrow{\partial_t}}{2} - H\right)|\Psi\rangle \tag{41}$$

$$\boxed{\langle\Phi|\Phi\rangle = -\frac{1}{2}\Re\big(\langle\Psi|\ \overrightarrow{\partial_t}\ \overrightarrow{\partial_t}\ |\Psi\rangle\big) + \frac{1}{2}\langle\Psi|\ \overleftarrow{\partial_t}\ \overrightarrow{\partial_t}\ |\Psi\rangle - 2\,\Im\big(\langle\Psi|\ \overleftarrow{\partial_t}\ H\ |\Psi\rangle\big) + \langle\Psi|H^2|\Psi\rangle} \tag{42}$$

Noting that:

$$\langle\alpha|\overleftarrow{\partial_t}|\beta\rangle = -\langle\alpha|\beta\rangle\,\frac{1}{2}\Big(\sum_p \dot{\alpha}_p\alpha_p^\star + \dot{\alpha}_p^\star\alpha_p - 2\beta_p\dot{\alpha}_p^\star\Big), \tag{43}$$

$$\langle\alpha|\overleftarrow{\partial_t}\ a_q^\dagger|\beta\rangle = \alpha_q^\star\,\langle\alpha|\overleftarrow{\partial_t}|\beta\rangle + \langle\alpha|\beta\rangle\,\dot{\alpha}_q^\star, \tag{44}$$

$$\langle\alpha|\overrightarrow{\partial_t}\ a_q^\dagger|\beta\rangle = \alpha_q^\star\,\langle\alpha|\overrightarrow{\partial_t}|\beta\rangle \tag{45}$$

$$\langle\alpha|a_q\overleftarrow{\partial_t}|\beta\rangle = \beta_q\,\langle\alpha|\overleftarrow{\partial_t}|\beta\rangle \tag{46}$$

we obtain

$$\begin{aligned}
\langle\Psi|\ \overleftarrow{\partial_t}\ H\ |\Psi\rangle = &\sum_{i,n,m} \dot{p}_{i,m}^\star p_{i,n}\,\langle z_{i,m}|z_{i,n}\rangle\left[\omega_i^{\mathrm{qb}} + \sum_{p=0}\omega_p z_{i,m}^{p\star}z_{i,n}^p + A(t)\sum_p O_{0p}(z_{im}^{p\star}+z_{in}^p)\right]\\
&+\sum_{i,j,n,m}\dot{p}_{i,m}^\star p_{j,n}\,\langle z_{i,m}|z_{j,n}\rangle\left[\sum_p g_{i,j}^p\big(z_{i,m}^{p\star}+z_{j,n}^p\big)\right]\\
&+\sum_{i,n,m} p_{i,m}^\star p_{i,n}\,\langle z_{i,m}|z_{i,n}\rangle\Bigg[-\frac{1}{2}\Big(\sum_p \dot{z}_{i,m}^p z_{i,m}^{p\star} + \dot{z}_{i,m}^{p\star}z_{i,m}^p - 2\dot{z}_{i,m}^{p\star}z_{i,n}^p\Big)\Big(\omega_i^{\mathrm{qb}} + \sum_p\omega_p z_{i,m}^{p\star}z_{in}^p + A(t)\sum_p O_{0p}(z_{im}^{p\star}+z_{in}^p)\Big)\\
&\qquad + \Big(\sum_p \omega_p\dot{z}_{im}^{p\star}z_{in}^p + A(t)\sum_p O_{0p}\dot{z}_{im}^{p\star}\Big)\Bigg]\\
&+\sum_{i,j,n,m} p_{i,m}^\star p_{j,n}\,\langle z_{i,m}|z_{j,n}\rangle\left[-\frac{1}{2}\Big(\sum_p \dot{z}_{i,m}^p z_{i,m}^{p\star} + \dot{z}_{i,m}^{p\star}z_{i,m}^p - 2\dot{z}_{i,m}^{p\star}z_{j,n}^p\Big)\Big(\sum_p g_{i,j}^p(z_{i,m}^{p\star}+z_{jn}^p)\Big) + \Big(\sum_p g_{ij}^p\dot{z}_{i,m}^{p\star}\Big)\right]
\end{aligned} \tag{47}$$

$$\begin{aligned}
\langle\Psi|H^2|\Psi\rangle = &\sum_{inm} p_{i,m}^\star p_{i,n}\,\langle z_{i,m}|z_{i,n}\rangle\Bigg[\Big(\omega_{\mathrm{qb}}^i + \sum_p \omega_p z_{im}^{p\star}z_{in}^p + A(t)\sum_p O_{0p}(z_{im}^{p\star}+z_{in}^p)\Big)^2\\
&\qquad + \sum_p \omega_p^2 z_{im}^{p\star}z_{in}^p + \sum_p \omega_p A(t)O_{0p}(z_{im}^{p\star}+z_{in}^p) + A^2(t)\sum_p O_{0p}^2\Bigg]\\
&+\sum_{i,j,n,m} p_{i,m}^\star p_{j,n}\,\langle z_{i,m}|z_{j,n}\rangle\Bigg[\Big(\sum_s n_{s,j}n_{s,i}\Big)\Big(\Big(\sum_p g_p(z_{i,m}^{p\star}+z_{jn}^p)\Big)^2 + \Big(\sum_p g_p^2\Big)\Big)\\
&\qquad + 2A(t)\Bigg(\Big(\sum_p g_p n_{ij}(z_{i,m}^{p\star}+z_{jn}^p)\Big)\Big(\sum_p O_{0p}(z_{i,m}^{p\star}+z_{jn}^p)\Big) + n_{ij}\Big(\sum_p O_{0p}g_p\Big)\Bigg)\\
&\qquad + (\omega_{\mathrm{qb}}^i + \omega_{\mathrm{qb}}^j)\Big(\sum_p g_{ij}^p(z_{im}^{p\star}+z_{j,n}^p)\Big) + 2\sum_{pq} g_{ji}^q\omega_p z_{jn}^p z_{im}^{p\star}\Big(z_{jn}^q + z_{im}^{q\star}\Big) + \sum_p g_{ij}^p\omega_p(z_{jn}^p + z_{im}^{p\star})\Bigg]
\end{aligned}$$

$$\begin{aligned}
\langle\Psi|\ \overleftarrow{\partial_t}\ \overrightarrow{\partial_t}\ |\Psi\rangle = &\sum_i\sum_{m,n}\langle z_{i,m}|z_{i,n}\rangle\Bigg[\dot{p}_{i,m}^*\dot{p}_{i,n} - \frac{1}{2}\dot{p}_{i,m}^* p_{i,n}\sum_p(\dot{z}_{i,n}^p z_{i,n}^{p*} + \dot{z}_{i,n}^{p*}z_{i,n}^p - 2\dot{z}_{i,n}^p z_{i,m}^{p*}) - \frac{1}{2}p_{i,m}^*\dot{p}_{i,n}\sum_p(\dot{z}_{i,m}^p z_{i,m}^{p*} + \dot{z}_{i,m}^{p*}z_{i,m}^p - 2\dot{z}_{i,m}^{p*}z_{i,n}^p)\\
&\qquad + p_{i,m}^\star p_{i,n}\Bigg[\sum_p \dot{z}_{i,m}^{p\star}\dot{z}_{i,n}^p + \frac{1}{4}\sum_{p,q}\Big(\dot{z}_{i,m}^p z_{i,m}^{p\star} + \dot{z}_{i,m}^{p*}z_{i,m}^p - 2\dot{z}_{i,m}^{p*}z_{i,n}^p\Big)\Big(\dot{z}_{i,n}^q z_{i,n}^{q\star} + \dot{z}_{i,n}^{q\star}z_{i,n}^q - 2\dot{z}_{i,n}^q z_{i,m}^{q\star}\Big)\Bigg]\Bigg]
\end{aligned}$$

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