A Calculations for the single-qubit case

A.1 Derivation of the basic commutation relations

Let A, B, and C be operators such that $[B, A] = C$. Then, if $[C, A] = 0$ it follows that $[B, A^n] = nCA^{n-1}$.

The proof is by induction:

$$\begin{aligned} [B, A^n] &= [B, AA^{n-1}] \\ &= A[B, A^{n-1}] + [B, A]A^{n-a} \\ \text{by I.H.} \rightarrow &= A(n-1)CA^{n-2} + CA^{n-1} \\ [C, A] = 0 \rightarrow &= (n-1)CA^{n-1} + CA^{n-1} \\ &= nCA^{n-1} \end{aligned} \tag{72}$$

From this, one can prove that $[B, e^A] = Ce^A$ also holds.

$$\begin{aligned} [B, e^A] &= \sum_{n=0} \frac{[B, A^n]^n}{n!} \\ &= [A, I] + \sum_{n=1} \frac{[B, A^n]^n}{n!} \\ &= \sum_{n=1} \frac{nCA^{n-1}}{n!} = C \sum_{n=1} \frac{A^{n-1}}{(n-1)!} \\ &= C \sum_{n=0} \frac{A^n}{n!} = Ce^A \end{aligned} \tag{73}$$

If we express the Polaron transform (Eq. (12)) as $U_P = \exp\{A\}$, we can apply the properties we just proved to arrive at the basic commutation relations in Eqs. (**??**) and (16).

$$\begin{aligned} &[b_k, A] = -\sigma^x \left(f_k[b_k, b_k^\dagger] - f_k^*[b_k, b_k] \right) = -f_k\sigma^x \rightarrow \\ &[b_k, U_P] = -f_k\sigma^x U_P \end{aligned} \tag{74}$$

$$\begin{aligned} &[b_k^\dagger, A] = -\sigma^x \left(f_k[b_k^\dagger, b_k^\dagger] - f_k^*[b_k^\dagger, b_k] \right) = -f_k\sigma^x \rightarrow \\ &[b_k^\dagger, U_P] = -f_k^*\sigma^x U_P \end{aligned} \tag{75}$$

A.2 Calculation of $\langle 00|\frac{\Delta}{2} \exp\left[2\sigma^x \sum_k f_k b_k^\dagger - f_k^* b_k\right] \sigma^z |00\rangle$

$$\begin{aligned} &\langle 00|\frac{\Delta}{2} \exp\left[2\sigma^x \sum_k f_k b_k^\dagger - f_k^* b_k\right] \sigma^z |00\rangle = -\frac{\Delta}{2} \langle 00|\exp\left[2\sigma^x \sum_k f_k b_k^\dagger - f_k^* b_k\right] |00\rangle = \\ &= -\frac{\Delta}{4} \left(\langle +\,0|\exp\left[2\sigma^x \sum_k f_k b_k^\dagger - f_k^* b_k\right] |+\,0\rangle + \langle -\,0|\exp\left[2\sigma^x \sum_k f_k b_k^\dagger - f_k^* b_k\right] |-\,0\rangle \right) \\ &= -\frac{\Delta}{4} \left(\langle 0|\exp\left[2 \sum_k f_k b_k^\dagger - f_k^* b_k\right] |0\rangle + \langle 0|\exp\left[-2 \sum_k f_k b_k^\dagger - f_k^* b_k\right] |0\rangle \right) = \star \end{aligned}$$

Now the Baker-Campbell-Hausdorff formula states that

$$e^{t(X+Y)} = e^{tX}\ e^{tY}\ e^{-\frac{t^2}{2}[X,Y]}\ e^{\frac{t^3}{6}(2[Y,[X,Y]]+[X,[X,Y]])} \dots \tag{76}$$

So we can write

$$\exp\left[\pm 2\sum_k f_k b_k^\dagger - f_k^* b_k\right] = \exp\left[-2\sum_k |f_k|^2\right]\exp\left[\pm 2\sum_k f_k b_k^\dagger\right]\exp\left[\mp 2\sum_k f_k^* b_k\right]. \tag{77}$$

From which it follows that

$$\langle 0|\exp\left[\pm 2\sum_k f_k b_k^\dagger\right]\exp\left[\mp 2\sum_k f_k^* b_k\right]|0\rangle = \left|\exp\left[\mp 2\sum_k f_k^* b_k\right]|0\rangle\right|^2 = 1. \tag{78}$$

We have used $b_k|0\rangle = 0 \equiv 0\,|0\rangle$, so $|0\rangle$ is an eigenstate of b_k with eigenvalue 0.

Continuing our calculation we arrive at the end result.

$$\star = -\frac{\Delta}{4}2\exp\left[-2\sum_k |f_k|^2\right] = -\frac{\Delta_r}{2} \tag{79}$$

A.3 Calculation of $\left\langle b_n^\dagger b_n\right\rangle$ for the GS of a single qubit

$$\begin{aligned}\left\langle b_n^\dagger b_n\right\rangle &= \langle GS|b_n^\dagger b_n|GS\rangle \\ &= \langle GS|\frac{1}{\sqrt{N}}\sum_k e^{ik(n-N/2)}b_k^\dagger\frac{1}{\sqrt{N}}\sum_p e^{-ip(n-N/2)}b_p|GS\rangle \\ &= \frac{1}{N}\sum_{k,p} e^{i(k-p)(n-N/2)}\,\langle 00|U_p^\dagger b_k^\dagger b_p U_p|00\rangle\end{aligned} \tag{80}$$

In order to continue, we must first calculate $U_p^\dagger b_k^\dagger b_p U_p$. Since we have already taken f_k as real in previous calculations, we assume it to be real here as well.

$$\begin{aligned}U_p^\dagger b_k^\dagger b_p U_p &= U_P^\dagger\left(b_k^\dagger[b_p,U_P] + [b_k^\dagger,U_P]b_p\right) + b_k^\dagger b_p \\ &= U_P^\dagger\left(-f_p\sigma^x b_k^\dagger U_P - f_k\sigma^x U_P b_p\right) + b_k^\dagger b_p \\ &= U_P^\dagger\left(-f_p\sigma^x[b_k^\dagger,U_P] - f_p\sigma^x U_P b_k^\dagger - f_k\sigma^x U_P b_p\right) + b_k^\dagger b_p \\ &= U_P^\dagger\left(U_P f_k f_p - f_p\sigma^x U_P b_k^\dagger - f_k\sigma^x U_P b_p\right) + b_k^\dagger b_p \\ &= f_k f_p - \sigma^x(f_p b_k^\dagger + f_k b_p) + b_k^\dagger b_p\end{aligned} \tag{81}$$

We are now equipped with the necessary ingredients to compute $\langle 00|U_p^\dagger b_k^\dagger b_p U_p|00\rangle$. Considering that the state $|00\rangle$ does not connect through the second and third terms, the mean value is just $f_k f_p$.

With that, we simply have

$$\left\langle b_n^\dagger b_n\right\rangle = \frac{1}{\sqrt{N}}\sum_k e^{ik(n-N/2)}f_k\frac{1}{\sqrt{N}}\sum_p e^{-ip(n-N/2)}f_p = f_n^* f_n = f_n^2. \tag{82}$$

A.4 Exponential localisation of the GS

We recall that (we should fix the sign convention)

$$f_k = \frac{g}{\sqrt{N}(\Delta_r + \omega_k)} \tag{83}$$

with

$$\omega_k = \omega_0 - 2\gamma \cos k \tag{84}$$

Noticing that

$$\mathcal{F}[\, e^{-\kappa|n-N/2|}\,] = \frac{1}{\sqrt{N}} \frac{1-e^{-2\kappa}}{1+e^{-2\kappa}+2e^{-\kappa}\cos k} \tag{85}$$

with *our* convention for the Fourier transform $\mathcal{F}[g(n)] = \sum_0^{N-1} e^{ik(n-N/2)}\, g(n)$. Therefore,

$$\mathcal{F}[\, e^{-\kappa|n-N/2|}\,] \sim f_k \tag{86}$$

with the identifications

$$\gamma \sim e^{-\kappa} \tag{87a}$$

$$\omega_0 + \Delta_r \sim 1 + e^{-2\kappa}, \tag{87b}$$

which yields

$$\kappa = \text{arccosh}\left(\frac{\omega_0 + \Delta_r}{2\gamma}\right). \tag{88}$$

A.5 Single qubit effective Hamiltonian

We have manipulated Eq. (23) to the form

$$H_P = \frac{\Delta}{2} \exp\left[2\sigma^x \sum_k f_k b_k^\dagger - f_k^* b_k\right] \sigma^z + \sum_k \omega_k b_k^\dagger b_k + \Delta_r \sigma^x \sum_k f_k \left(b_k^\dagger + b_k\right) + E_{ZP}. \tag{89}$$

We can further simplify it by expanding the exponential term. Making use of the BCH formula in Eq. (76) and taking f_k real we get

$$\exp\left[2\sigma^x \sum_k f_k b_k^\dagger - f_k b_k\right] = \exp\left[-2\sum_k f_k^2\right] \exp\left[2\sigma^x \sum_k f_k b_k^\dagger\right] \exp\left[-2\sigma^x \sum_k f_k b_k\right]. \tag{90}$$

A power series expansions of the non constant terms gives

$$\exp\left[2\sigma^x \sum_k f_k b_k^\dagger\right] = 1 + 2\sigma^x \sum_k f_k b_k^\dagger + \ldots, \tag{91}$$

$$\exp\left[-2\sigma^x \sum_k f_k b_k\right] = 1 - 2\sigma^x \sum_k f_k b_k + \ldots. \tag{92}$$

Ignoring higher order terms the right hand side of Eq. (90) becomes

$$\exp\left[-2\sum_k f_k^2\right] \left(1 + 2\sigma^x \sum_k f_k \left(b_k^\dagger - b_k\right) - 4 \sum_{k,p} f_k f_p b_k^\dagger b_p\right). \tag{93}$$

Reintroducing this result in H_{eff} yields

$$\begin{aligned} H_{\text{eff}} = &\frac{\Delta_r}{2}\sigma^z + \Delta_r \sigma^x \sigma^z \sum_k f_k \left(b_k^\dagger - b_k\right) - 2\Delta_r \sum_{k,p} f_k f_p b_k^\dagger b_p \\ &+ \sum_k \omega_k b_k^\dagger b_k + \Delta_r \sigma^x \sum_k f_k \left(b_k^\dagger + b_k\right) + E_{ZP}. \end{aligned} \tag{94}$$

Considering that $\sigma^x\sigma^z + \sigma^x = 2\sigma^-$ and $-\sigma^x\sigma^z + \sigma^x = 2\sigma^+$ we can combine the second and second-to-last terms to arrive at the final expression for H_{eff}

$$H_{\text{eff}} = \frac{\Delta_r}{2}\sigma^z + \sum_k \omega_k b_k^\dagger b_k + 2\Delta_r \sum_k f_k \left(\sigma^- b_k^\dagger - \sigma^+ b_k\right) - 2\Delta_r \sum_{k,p} f_k f_p b_k^\dagger b_p + E_{ZP}. \tag{95}$$

A.6 Calculation of $\left\langle b_n^\dagger b_n \right\rangle$ for the SEBS of a single qubit

The SEBS will be a state of the form

$$|v\rangle = \lambda_0 |1\rangle |0\rangle + \sum_k \lambda_k |0\rangle |1_k\rangle . \quad (96)$$

Thus

$$\begin{aligned} \left\langle b_n^\dagger b_n \right\rangle &= \langle v|b_n^\dagger b_n|v\rangle \\ &= \langle v|\frac{1}{\sqrt{N}}\sum_k e^{ik(n-N/2)} b_k^\dagger \frac{1}{\sqrt{N}}\sum_p e^{-ip(n-N/2)} b_p|v\rangle \\ &= \frac{1}{N}\sum_{k,p} e^{i(k-p)(n-N/2)} \langle v|U_p^\dagger b_k^\dagger b_p U_p|v\rangle . \end{aligned} \quad (97)$$

In App. A.3 we saw that $U_p^\dagger b_k^\dagger b_p U_p = f_k f_p - \sigma^x(f_p b_k^\dagger + f_k b_p) + b_k^\dagger b_p$. The first term is constant so $|v\rangle$ connects entirely yielding $f_k f_p$. The last term only connects the bosonic part of $|v\rangle$ to give $\lambda_k \lambda_p$. Finally, the second term cross-connects the two components of $|v\rangle$ resulting in $\lambda_0 f_p \lambda_k^* + \lambda_0 f_k \lambda_p$. Reintroducing these partial results into Eq. (117) one has

$$\left\langle b_n^\dagger b_n \right\rangle = f_n^2 + \lambda_n^2 + \lambda_0 f_n^* \lambda_n^* + \lambda_0 f_n \lambda_n = f_n^2 + \lambda_n^2 + 2\lambda_0 \,\mathrm{Re}\{f_n \lambda_n\}. \quad (98)$$

B Calculations for the two-qubit case

B.1 Derivation of the basic commutation relations

Recycling much od the work done in Ap. A.1 we simply see that

$$\begin{aligned} &[b_k, A_j] = -\sigma_j^x \left(f_k e^{ikx_j}[b_k, b_k^\dagger] - f_k e^{-ikx_j}[b_k, b_k]\right) = -\sigma^x f_k e^{ikx_j} \rightarrow \\ &[b_k, U_j] = -\sigma^x f_k e^{ikx_j} U_j \quad (99) \\ &[b_k^\dagger, A_j] = -\sigma_j^x \left(f_k e^{ikx_j}[b_k^\dagger, b_k^\dagger] - f_k e^{-ikx_j}[b_k^\dagger, b_k]\right) = -\sigma^x f_k e^{-ikx_j} \rightarrow \\ &[b_k^\dagger, U_j] = -\sigma^x f_k e^{-ikx_j} U_j. \quad (100) \end{aligned}$$

B.2 Calculation of H_I

In an attempt to lighten notation we have omitted the summation signs ($\sum$) in the following calculation. They will be reintroduced when we present the final result. It must be understood that there is summation over all indexes present, for instance

$$\sigma_j^x c_k \left(b_k^\dagger e^{ikx_j} + b_k e^{-ikx_j}\right) \equiv \sum_j \sigma_j^x \sum_k c_k \left(b_k^\dagger e^{ikx_j} + b_k e^{-ikx_j}\right). \quad (101)$$

We thus have

$$U_P^\dagger H_I U_P = U_2^\dagger U_1^\dagger \left(H_I^1 + H_I^2\right) U_1 U_2, \quad (102)$$

we can focus on H_I^1 and the results will be perfectly extensible to H_I^2.

Hence,

$$U_2^\dagger U_1^\dagger H_I^1 U_1 U_2 = U_2^\dagger U_1^\dagger \sigma_1^x c_k \left(b_k^\dagger e^{ikx_1} + b_k e^{-ikx_1}\right) U_1 U_2$$

$$
\begin{aligned}
&= U_2^\dagger \left(\sigma_1^x c_k \left(-\sigma_1^x e^{ikx_1} f_k e^{-ikx_1} - \sigma_1^x e^{-ikx_1} f_k e^{ikx_1}\right) + H_I^1\right) U_2 \\
&= U_2^\dagger \left(-2c_k f_k + H_I^1\right) U_2 = -2c_k f_k + U_2^\dagger H_I^1 U_2 \\
&= -2c_k f_k + U_2^\dagger \left(\sigma_1^x c_k \left(b_k^\dagger e^{ikx_1} + b_k e^{-ikx_1}\right)\right) U_2 \\
&= -2c_k f_k + \sigma_1^x c_k \left(-\sigma_2^x e^{ikx_1} f_k e^{-ikx_2} - \sigma_2^x e^{-ikx_1} f_k e^{ikx_2}\right) + H_I^1 \\
&= -2c_k f_k - 2\sigma_1^x \sigma_2^x c_k f_k \cos(kx) + H_I^1.
\end{aligned}
\tag{103}
$$

Likewise,

$$
U_2^\dagger U_1^\dagger H_I^2 U_1 U_2 = -2c_k f_k - 2\sigma_1^x \sigma_2^x c_k f_k \cos(kx) + H_I^2. \tag{104}
$$

And finally,

$$
U_P^\dagger H_I U_P = -4\sum_k c_k f_k - 4\sigma_1^x \sigma_2^x \sum_k c_k f_k \cos(kx) + H_I. \tag{105}
$$

B.3 Calculation of H_B

Much like in App. B.2 we have omitted the summation signs for the calculation.

$$
\begin{aligned}
U_P^\dagger H_B U_P &= U_2^\dagger U_1^\dagger \omega_k b_k^\dagger b_k U_1 U_2 \\
&= \omega_k U_2^\dagger \left(U_1^\dagger \left(b_k^\dagger [b_k, U_1] + [b_k^\dagger, U_1] b_k\right) + H_B/\omega_k\right) \\
&= \omega_k U_2^\dagger \left(U_1^\dagger \left(-\sigma_1^x b_k^\dagger f_k e^{ikx_1} U_1 - \sigma f_k e^{-ikx_1} U_1 b_k\right) + H_B/\omega_k\right) U_2 \\
&= \omega_k U_2^\dagger \left(U_1^\dagger \left(-\sigma_1^x f_k e^{ikx_1} \left(U_1 b_k^\dagger - \sigma_1^x f_k e^{-ikx_1} U_1\right) - \sigma_1^x f_k e^{-ikx_1} U_1 b_k\right) + H_B/\omega_k\right) U_2 \\
&= \omega_k U_2^\dagger \left(-\sigma_1^x f_k \left(b_k^\dagger e^{ikx_1} + b_k e^{-ikx_1}\right) + f_k^2 + H_B/\omega_k\right) U_2 \\
&= H_B + \omega_k \Big(2f_k^2 - \sigma_1^x f_k \left(b_k^\dagger e^{ikx_1} + b_k e^{-ikx_1}\right) - \sigma_2^x f_k \left(b_k^\dagger e^{ikx_2} + b_k e^{-ikx_2}\right) \\
&\qquad + U_2^\dagger \left[-\sigma_1^x f_k \left(b_k^\dagger e^{ikx_1} + b_k e^{-ikx_1}\right), U_2\right]\Big) \\
&= H_B + \omega_k \Big(2f_k^2 - \sigma_j^x f_k \left(b_k^\dagger e^{ikx_j} + b_k e^{-ikx_j}\right) \\
&\qquad - \sigma_1^x f_k \left(-\sigma_2^x e^{ikx_1} f_k e^{-ikx_2} - \sigma_2^x e^{-ikx_1} f_k e^{ikx_2}\right)\Big) \\
&= \omega_k \left(2f_k^2 - \sigma_j^x f_k \left(b_k^\dagger e^{ikx_j} + b_k e^{-ikx_j}\right) + 2\sigma_1^x \sigma_2^x f_k^2 \cos(k(x_2 - x_1))\right) + H_B
\end{aligned}
\tag{106}
$$

So finally,

$$
\begin{aligned}
U_P^\dagger H_B U_P = 2\sum_k \omega_k f_k^2 + 2\sigma_1^x \sigma_2^x \sum_k \omega_k f_k^2 \cos(kx) \\
- \sum_j \sigma_j^x \sum_k \omega_k f_k \left(b_k^\dagger e^{ikx_j} + b_k e^{-ikx_j}\right) + \sum_k \omega_k b_k^\dagger b_k.
\end{aligned}
\tag{107}
$$

B.4 Calculation of the minimal value of f_k

The explicit dependence of $\bar{E}_{GS}$ with f_k is

$$
\bar{E}_{GS} = -E + 2\sum_k f_k(\omega_k f_k - 2c_k) = -\sqrt{\Delta_r^2 + J^2} + 2\sum_k f_k(\omega_k f_k - 2c_k)
$$

$$= -\sqrt{4\left(\sum_k f_k(2c_k - \omega_k f_k)\cos(kx)\right)^2 + \Delta^2 \exp\left[-4\sum_k f_k^2\right]} + 2\sum_k f_k(\omega_k f_k - 2c_k). \tag{108}$$

Thus

$$\begin{aligned}
&\frac{\partial \bar{E}_{GS}}{\partial f_k} = -\frac{4J(2c_k - 2\omega_k f_k)\cos(kx)) - 8f_k\Delta_r^2}{2E} + 2(2\omega_k f_k - 2_c k) = 0 \rightarrow \\
&-\frac{J(c_k - \omega_k f_k)\cos(kx) - f_k\Delta_r^2}{E} + (\omega_k f_k - c_k) = 0 \rightarrow \\
&E(\omega_k f_k - c_k) = J(c_k - \omega_k f_k)\cos(kx) - f_k\Delta_r^2 \rightarrow \\
&E\omega_k f_k - Ec_k = Jc_k\cos(kx) - J\omega_k\cos(kx)f_k - f_k\Delta_r^2 \rightarrow \\
&\left(E\omega_k + J\omega_k\cos(kx) + \Delta_r^2\right) f_k = Ec_k + Jc_k\cos(kx) \rightarrow \\
&f_k = c_k\frac{E + J\cos(kx)}{E\omega_k + J\omega_k\cos(kx) + \Delta_r^2}
\end{aligned} \tag{109}$$

B.5 Calculation of $\left\langle b_n^\dagger b_n \right\rangle$ for the GS of the two-qubit scenario

The ground state is

$$|GS\rangle = (\alpha\,|00\rangle + \beta\,|11\rangle)\,|0\rangle \tag{110}$$

Thus

$$\begin{aligned}
\left\langle b_n^\dagger b_n \right\rangle &= \langle GS|b_n^\dagger b_n|GS\rangle \\
&= \langle GS|\frac{1}{\sqrt{N}}\sum_k e^{ik(n-N/2)}b_k^\dagger \frac{1}{\sqrt{N}}\sum_p e^{-ip(n-N/2)}b_p|GS\rangle \\
&= \frac{1}{N}\sum_{k,p} e^{i(k-p)(n-N/2)}\,\langle GS|U_p^\dagger b_k^\dagger b_p U_p|GS\rangle\,.
\end{aligned} \tag{111}$$

We must now calculate $U_p^\dagger b_k^\dagger b_p U_p$ in the two-qubit case.

$$\begin{aligned}
U_p^\dagger b_k^\dagger b_p U_p &= U_2^\dagger U_1^\dagger b_k^\dagger b_p U_1 U_2 \\
&= U_2^\dagger U_1^\dagger \left(\left(b_k^\dagger[b_p, U_1] + [b_k^\dagger, U_1]b_p\right) + b_k^\dagger b_p\right) U_2 \\
&= U_2^\dagger U_1^\dagger \left(\left(-f_p e^{ipx_1}\sigma_1^x b_k^\dagger U_1 - f_k e^{-ikx_1}\sigma_1^x U_1 b_p\right) + b_k^\dagger b_p\right) U_2 \\
&= U_2^\dagger \left(\left(-f_p e^{ipx_1}\sigma_1^x\right)\left(-f_k e^{-ikx_1}\sigma_1^x\right) - f_p e^{ipx_1}\sigma_1^x b_k^\dagger - f_k e^{-ikx_1}\sigma_1^x b_p + b_k^\dagger b_p\right) U_2 \\
&= U_2^\dagger \left(f_k f_p e^{-ikx_1}e^{ipx_1} - f_p e^{ipx_1}\sigma_1^x b_k^\dagger - f_k e^{-ikx_1}\sigma_1^x b_p + b_k^\dagger b_p\right) U_2 \\
&= f_k f_p e^{-ikx_1}e^{ipx_1} + f_k f_p e^{-ikx_2}e^{ipx_2} \\
&\quad - f_p e^{ipx_1}\sigma_1^x b_k^\dagger - f_k e^{-ikx_1}\sigma_1^x b_p \\
&\quad - f_p e^{ipx_2}\sigma_2^x b_k^\dagger - f_k e^{-ikx_2}\sigma_2^x b_p \\
&\quad + b_k^\dagger b_p + \left[-f_p e^{ipx_1}\sigma_1^x b_k^\dagger, U_2\right] + \left[-f_k e^{-ikx_1}\sigma_1^x b_p, U_2\right]
\end{aligned}$$

The last two terms give,

$$= -f_p e^{ipx_1}\sigma_1^x\left(-\sigma_2^x f_k e^{-ikx_2}\right) - f_k e^{-ikx_1}\sigma_1^x\left(-\sigma_2^x f_p e^{ipx_2}\right)$$

$$= \sigma_1^x \sigma_2^x f_p f_k e^{ipx_1} e^{-ikx_2} + \sigma_1^x \sigma_2^x f_p f_k e^{ipx_2} e^{-ikx_1}.$$

Putting everything together one has

$$\begin{aligned} U_p^\dagger b_k^\dagger b_p U_p = & f_k f_p e^{-ikx_1} e^{ipx_1} + f_k f_p e^{-ikx_2} e^{ipx_2} \\ & - \sum_j \sigma_j^x \left(f_p e^{ipx_j} b_k^\dagger + f_k e^{-ikx_j} b_p \right) \\ & + \sigma_1^x \sigma_2^x f_p f_k \left(e^{ipx_1} e^{-ikx_2} + e^{ipx_2} e^{-ikx_1} \right) \\ & + b_k^\dagger b_p \end{aligned} \tag{112}$$

The ground state has no photons, so it only connects through the first and second-to-last terms of $U_p^\dagger b_k^\dagger b_p U_p$. The first connects completely, while the other cross-connects the spin terms $|00\rangle$ and $|11\rangle$, this yields

$$\begin{aligned} \langle GS|U_p^\dagger b_k^\dagger b_p U_p|GS\rangle = & f_k f_p e^{-ikx_1} e^{ipx_1} + f_k f_p e^{-ikx_2} e^{ipx_2} \\ & + 2\alpha\beta f_p f_k \left(e^{ipx_1} e^{-ikx_2} + e^{ipx_2} e^{-ikx_1} \right). \end{aligned} \tag{113}$$

Completing the Fourier transform one finally arrives at

$$\left\langle b_n^\dagger b_n \right\rangle = |f_{n,1}|^2 + |f_{n,2}|^2 + 4\alpha\beta \,\mathrm{Re}\{f_{n,1} f_{n,2}^*\}. \tag{114}$$

Where $f_{n,1}$ is the fourier transform of $f_{k,1}$, defined as

$$f_{k,1} = f_k e^{ikx_1}. \tag{115}$$

B.6 Calculation of $\left\langle b_n^\dagger b_n \right\rangle$ for the bound states of the two-qubit scenario

The SEBS will be states of the form

$$|v\rangle = \lambda_0 |01\rangle |0\rangle + \lambda_1 |10\rangle |0\rangle + \sum_k \lambda_k (\alpha |00\rangle + \beta |11\rangle) |1_k\rangle. \tag{116}$$

Thus

$$\begin{aligned} \left\langle b_n^\dagger b_n \right\rangle &= \langle v|b_n^\dagger b_n|v\rangle \\ &= \langle v|\frac{1}{\sqrt{N}} \sum_k e^{ik(n-N/2)} b_k^\dagger \frac{1}{\sqrt{N}} \sum_p e^{-ip(n-N/2)} b_p|v\rangle \\ &= \frac{1}{N} \sum_{k,p} e^{i(k-p)(n-N/2)} \langle v|U_p^\dagger b_k^\dagger b_p U_p|v\rangle. \end{aligned} \tag{117}$$

We saw in App. B.5 that

$$\begin{aligned} U_p^\dagger b_k^\dagger b_p U_p = & f_k f_p e^{-ikx_1} e^{ipx_1} + f_k f_p e^{-ikx_2} e^{ipx_2} \\ & - \sum_j \sigma_j^x \left(f_p e^{ipx_j} b_k^\dagger + f_k e^{-ikx_j} b_p \right) \\ & + \sigma_1^x \sigma_2^x f_p f_k \left(e^{ipx_1} e^{-ikx_2} + e^{ipx_2} e^{-ikx_1} \right) \\ & + b_k^\dagger b_p. \end{aligned} \tag{118}$$

Contrary to what happened with the GS, all terms must now be considered because the SEBS connect through them all in one way or another. Thus, we must study each term individually.

The first two are trivial, as the connect completely, so they will not be discussed.

The second term is more interesting. Through

$$-\sum_j \sigma_j^x \left(f_p e^{ipx_j} b_k^\dagger + f_k e^{-ikx_j} b_p\right), \tag{119}$$

the term $\lambda_0 |01\rangle |0\rangle$ in $|v\rangle$ becomes $-\lambda_0 f_{p,1} |11\rangle |1_k\rangle - \lambda_0 f_{p,2} |00\rangle |1_k\rangle$, which connects with $\lambda_k (\alpha |00\rangle + \beta |11\rangle) |1_k\rangle$ to yield $-\lambda_0\lambda_k (\beta f_{p,1} + \alpha f_{p,2})$. The term $\lambda_1 |10\rangle |0\rangle$ in $|v\rangle$ becomes $-\lambda_1 f_{p,1} |11\rangle |1_k\rangle - \lambda_1 f_{p,2} |00\rangle |1_k\rangle$, which connects with $\lambda_k (\alpha |00\rangle + \beta |11\rangle) |1_k\rangle$ to yield $-\lambda_1\lambda_k (\alpha f_{p,1} + \beta f_{p,2})$. Naturally, the term $(\alpha |00\rangle + \beta |11\rangle) \sum_k \lambda_k |1_k\rangle$ connects with both $\lambda_0 |01\rangle |0\rangle$ and $\lambda_1 |10\rangle |0\rangle$ to yield the complex conjugate of the terms that we just calculated in the opposite direction.

Through the third term,

$$+\sigma_1^x \sigma_2^x f_p f_k \left(e^{ipx_1} e^{-ikx_2} + e^{ipx_2} e^{-ikx_1}\right), \tag{120}$$

the term $\lambda_0 |01\rangle |0\rangle$ in $|v\rangle$ becomes $\lambda_0 \left(f_{p,1} f_{k,2}^* + f_{p,2} f_{k,1}^*\right) |10\rangle |0\rangle$, which connects with $\lambda_1 |10\rangle |0\rangle$ to yield $\lambda_0\lambda_1 \left(f_{p,1} f_{k,2}^* + f_{p,2} f_{k,1}^*\right)$. Naturally, the term $\lambda_1 |10\rangle |0\rangle$ in $|v\rangle$ becomes $\lambda_1 \left(f_{p,1} f_{k,2}^* + f_{p,2} f_{k,1}^*\right) |01\rangle |0\rangle$, which connects with $\lambda_0 |01\rangle |0\rangle$ to yield $\lambda_0\lambda_1 \left(f_{p,1} f_{k,2}^* + f_{p,2} f_{k,1}^*\right)$, the complex conjugate of its counterpart. Lastly, the term $(\alpha |00\rangle + \beta |11\rangle) \sum_k \lambda_k |1_k\rangle$ becomes $(\alpha |11\rangle + \beta |00\rangle) \sum_k \lambda_k |1_k\rangle \left(f_{p,1} f_{k,2}^* + f_{p,2} f_{k,1}^*\right)$, and connects with $(\alpha |00\rangle + \beta |11\rangle) \sum_k \lambda_k |1_k\rangle$ to yield $2\alpha\beta \left(1 - \lambda_0^2 - \lambda_1^2\right) (\alpha |00\rangle + \beta |11\rangle) \left(f_{p,1} f_{k,2}^* + f_{p,2} f_{k,1}^*\right)$.

Finally, the term $b_k^\dagger b_p$ connects the p^{th} and k^{th} photonic terms to yield $\lambda_k^* \lambda_p$.

Summarizing, we have

$$\begin{aligned}
\langle v|U_p^\dagger b_k^\dagger b_p U_p|v\rangle = &\left(f_{k,1}^* f_{p,2} + f_{k,2}^* f_{p,1}\right) \\
&- \lambda_0\lambda_k \left(\beta f_{p,1} + \alpha f_{p,2}\right) - \lambda_1\lambda_k \left(\alpha f_{p,1} + \beta f_{p,2}\right) \\
&- \lambda_0\lambda_p \left(\beta f_{k,1}^* + \alpha f_{k,2}^*\right) - \lambda_1\lambda_p \left(\alpha f_{k,1}^* + \beta f_{k,2}^*\right) \\
&+ \lambda_0\lambda_1 \left(f_{p,1} f_{k,2}^* + f_{p,2} f_{k,1}^*\right) \\
&+ 2\alpha\beta \left(1 - \lambda_0^2 - \lambda_1^2\right) (\alpha |00\rangle + \beta |11\rangle) \left(f_{p,1} f_{k,2}^* + f_{p,2} f_{k,1}^*\right) \\
&+ \lambda_k^* \lambda_p.
\end{aligned} \tag{121}$$

Completing the Fourier transform, one arrives at

$$\begin{aligned}
\left\langle b_n^\dagger b_n \right\rangle = &|f_{n,1}|^2 + |f_{n,2}|^2 \\
&- 2\lambda_0 \operatorname{Re}\{\lambda_n^* \left(\beta f_{n,1} + \alpha f_{n,2}\right)\} \\
&- 2\lambda_1 \operatorname{Re}\{\lambda_n^* \left(\alpha f_{n,1} + \beta f_{n,2}\right)\} \\
&+ 4\lambda_0\lambda_1 \operatorname{Re}\left\{f_{n,1} f_{n,2}^*\right\} \\
&+ 4\alpha\beta \left(1 - \lambda_0^2 - \lambda_1^2\right) \operatorname{Re}\left\{f_{n,1} f_{n,2}^*\right\} \\
&+ |\lambda_n|^2
\end{aligned} \tag{122}$$

Where $f_{n,1}$ is the fourier transform of $f_{k,1}$, defined as

$$f_{k,1} = f_k e^{ikx_1}. \tag{123}$$

C Code

All numerical calculations performed in this End-of-Degree Thesis were based on proprietary code developed by the author that can be found here.