I. MODEL HAMILTONIAN IN MOMENTUM SPACE

Let us consider our three-dimensional bosonic Hamiltonian. Here, the bosonic tight-binding Hamiltonian reads

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{int},$$

$$\hat{\mathcal{H}}_0 = \sum_{l,l'}\sum_{\boldsymbol{k}} h^{l,l'}_{\boldsymbol{k}} \hat{a}^\dagger_{\boldsymbol{k},l}\hat{a}_{\boldsymbol{k},l'} - \mu_0 \sum_{l}\sum_{\boldsymbol{k}} \hat{a}^\dagger_{\boldsymbol{k},l}\hat{a}_{\boldsymbol{k},l},$$

$$\hat{\mathcal{H}}^{\mathsf{D_{4h}}}_{int} = \frac{1}{2}\sum_{\boldsymbol{r}}\sum_{l}(u+w)\hat{a}^\dagger_{\boldsymbol{r},l}\hat{a}^\dagger_{\boldsymbol{r},l}\hat{a}_{\boldsymbol{r},l}\hat{a}_{\boldsymbol{r},l} - \frac{1}{2}\sum_{\boldsymbol{r}}\sum_{l} v\hat{a}^\dagger_{\boldsymbol{r},l}\hat{a}^\dagger_{\boldsymbol{r},l}\hat{a}_{\boldsymbol{r},\bar{l}}\hat{a}_{\boldsymbol{r},\bar{l}} + \sum_{\boldsymbol{r}}(u+v-w)\,\hat{a}^\dagger_{\boldsymbol{r},1}\hat{a}^\dagger_{\boldsymbol{r},2}\hat{a}_{\boldsymbol{r},1}\hat{a}_{\boldsymbol{r},2}.$$

where $\hat{a}^\dagger_{\boldsymbol{k},l}$ ($\hat{a}_{\boldsymbol{k},l}$) creates (annihilates) a boson with momentum $\boldsymbol{k} = (k_x, k_y, k_z)$ of the degenerate component $l \in \{1,2\}$. For the hopping Hamiltonian we assume a $\mathsf{D_{4h}}$ three-dimensional tetragonal system with

$$\hat{\mathcal{H}}_0 = \sum_{l,l'}\sum_{\boldsymbol{k}} \delta_{ll'} \underbrace{\left(\mathsf{d}_{\parallel}\left(2-\cos(k_x a)-\cos(k_y a)\right)+\mathsf{d}_z\left(1-\cos(k_z c)\right)\right)}_{f^{A_{1g}}_{\boldsymbol{k}}} \hat{a}^\dagger_{\boldsymbol{k},l}\hat{a}_{\boldsymbol{k},l'} - \mu_0 \sum_{l}\sum_{\boldsymbol{k}} \hat{a}^\dagger_{\boldsymbol{k},l}\hat{a}_{\boldsymbol{k},l},$$

$$\hat{a}_{\boldsymbol{r},l} = \frac{1}{\sqrt{N_x N_y N_z}}\sum_{\boldsymbol{k}} e^{-\mathrm{i}\boldsymbol{r}\boldsymbol{k}}\hat{a}_{\boldsymbol{k},l}$$

The (on–site) interacting Hamiltonian reads

$$\hat{\mathcal{H}}^{\mathsf{D_{4h}}}_{int} = \frac{1}{2}\sum_{\boldsymbol{r}}\sum_{l}(u+w)\hat{a}^\dagger_{\boldsymbol{r},l}\hat{a}^\dagger_{\boldsymbol{r},l}\hat{a}_{\boldsymbol{r},l}\hat{a}_{\boldsymbol{r},l} - \frac{1}{2}\sum_{\boldsymbol{r}}\sum_{l} v\hat{a}^\dagger_{\boldsymbol{r},l}\hat{a}^\dagger_{\boldsymbol{r},l}\hat{a}_{\boldsymbol{r},\bar{l}}\hat{a}_{\boldsymbol{r},\bar{l}} + \sum_{\boldsymbol{r}}(u+v-w)\,\hat{a}^\dagger_{\boldsymbol{r},1}\hat{a}^\dagger_{\boldsymbol{r},2}\hat{a}_{\boldsymbol{r},1}\hat{a}_{\boldsymbol{r},2},$$

which we aim to decouple in the channels

$$n_{l,l'}(\boldsymbol{r}) = \langle \hat{a}^\dagger_{\boldsymbol{r},l}\hat{a}_{\boldsymbol{r},l'}\rangle, \qquad x_{l,l'}(\boldsymbol{r}) = \langle \hat{a}_{\boldsymbol{r},l}\hat{a}_{\boldsymbol{r},l'}\rangle,$$

$$x^*_{l,l'}(\boldsymbol{r}) = \langle \hat{a}^\dagger_{\boldsymbol{r},l}\hat{a}^\dagger_{\boldsymbol{r},l'}\rangle,$$

or in momentum space

$$\sum_{\boldsymbol{q}} e^{-\mathrm{i}\boldsymbol{r}\boldsymbol{q}} n_{l,l'}(\boldsymbol{q}) = \frac{1}{N_x N_y N_z}\sum_{\boldsymbol{q}} e^{-\mathrm{i}\boldsymbol{r}\boldsymbol{q}}\sum_{\boldsymbol{k}_1}\langle \hat{a}^\dagger_{\boldsymbol{k}_1-\boldsymbol{q},l}\hat{a}_{\boldsymbol{k}_1,l'}\rangle \sum_{\boldsymbol{q}} e^{-\mathrm{i}\boldsymbol{r}\boldsymbol{q}} x_{l,l'}(\boldsymbol{q}) = \frac{1}{N_x N_y N_z}\sum_{\boldsymbol{q}} e^{-\mathrm{i}\boldsymbol{r}\boldsymbol{q}}\sum_{\boldsymbol{k}_1}\langle \hat{a}_{-\boldsymbol{k}_1+\boldsymbol{q},l}\hat{a}_{\boldsymbol{k}_1,l'}\rangle$$

$$n_{l,l'}(\boldsymbol{q}) = \frac{1}{N_x N_y N_z}\sum_{\boldsymbol{k}}\langle \hat{a}^\dagger_{\boldsymbol{k}-\boldsymbol{q},l}\hat{a}_{\boldsymbol{k},l'}\rangle, x_{l,l'}(\boldsymbol{q}) = \frac{1}{N_x N_y N_z}\sum_{\boldsymbol{k}}\langle \hat{a}_{-\boldsymbol{k}+\boldsymbol{q},l}\hat{a}_{\boldsymbol{k},l'}\rangle,$$

$$x^*_{l,l'}(\boldsymbol{q}) = \frac{1}{N_x N_y N_z}\sum_{\boldsymbol{k}}\langle \hat{a}^\dagger_{-\boldsymbol{k}+\boldsymbol{q},l}\hat{a}^\dagger_{\boldsymbol{k},l'}\rangle,$$

and it holds

$$n^*_{1,2}(\boldsymbol{q}) = \frac{1}{N_x N_y N_z}\sum_{\boldsymbol{k}}\langle \hat{a}^\dagger_{\boldsymbol{k}-\boldsymbol{q},1}\hat{a}_{\boldsymbol{k},2}\rangle^* = \frac{1}{N_x N_y N_z}\sum_{\boldsymbol{k}}\langle \hat{a}^\dagger_{\boldsymbol{k},2}\hat{a}_{\boldsymbol{k}-\boldsymbol{q},1}\rangle = n_{2,1}(-\boldsymbol{q}),$$

$$x^*_{l,l'}(\boldsymbol{q}) = \frac{1}{N_x N_y N_z}\sum_{\boldsymbol{k}}\langle \hat{a}^\dagger_{-\boldsymbol{k}+\boldsymbol{q},l'}\hat{a}^\dagger_{\boldsymbol{k},l}\rangle = x^*_{l,l'}(\boldsymbol{q}),$$

$$n^*_{l,l}(\boldsymbol{q}) = \frac{1}{N_x N_y N_z}\sum_{\boldsymbol{k}}\langle \hat{a}^\dagger_{\boldsymbol{k}-\boldsymbol{q},l}\hat{a}_{\boldsymbol{k},l}\rangle^* = \frac{1}{N_x N_y N_z}\sum_{\boldsymbol{k}}\langle \hat{a}^\dagger_{\boldsymbol{k},l}\hat{a}_{\boldsymbol{k}-\boldsymbol{q},l}\rangle = n_{l,l}(-\boldsymbol{q}).$$

Now, we mean-field decouple the interaction contribution in all of the particle-hole $\langle \hat{a}^{\dagger}_{\boldsymbol{r},l}\hat{a}_{\boldsymbol{r}',l'}\rangle$ and particle-particle $\langle \hat{a}_{\boldsymbol{r},l}\hat{a}_{\boldsymbol{r}',l'}\rangle$ channels, leading to

$$
\begin{aligned}
\sum_{\boldsymbol{r}} \hat{a}^{\dagger}_{\boldsymbol{r},l_1}\hat{a}^{\dagger}_{\boldsymbol{r},l_2}\hat{a}_{\boldsymbol{r},l_3}\hat{a}_{\boldsymbol{r},l_4} \rightarrow{}& \frac{1}{6}\sum_{\boldsymbol{k},\boldsymbol{k}'}\Bigg(n_{l_2,l_4}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},l_1}\hat{a}_{\boldsymbol{k}',l_3} + n_{l_1,l_3}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},l_2}\hat{a}_{\boldsymbol{k}',l_4} + n_{l_2,l_3}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},l_1}\hat{a}_{\boldsymbol{k}',l_4} \\
&+ n_{l_1,l_4}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},l_2}\hat{a}_{\boldsymbol{k}',l_3}\Bigg) + \frac{1}{6}\sum_{\boldsymbol{k},\boldsymbol{q}}\left(x_{l_3,l_4}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},l_1}\hat{a}^{\dagger}_{-\boldsymbol{k}',l_2} + x^{*}_{l_1,l_2}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}_{\boldsymbol{k},l_3}\hat{a}_{-\boldsymbol{k}',l_4}\right) \\
&- \frac{1}{6}\Bigg(\delta_{l_3,l_2}\sum_{\boldsymbol{k}}\hat{a}^{\dagger}_{\boldsymbol{k},l_1}\hat{a}_{\boldsymbol{k},l_4} + \delta_{l_3,l_1}\sum_{\boldsymbol{k}}\hat{a}^{\dagger}_{\boldsymbol{k},l_2}\hat{a}_{\boldsymbol{k},l_4} + \delta_{l_4,l_2}\sum_{\boldsymbol{k}}\hat{a}^{\dagger}_{\boldsymbol{k},l_1}\hat{a}_{\boldsymbol{k},l_3} + \delta_{l_4,l_1}\sum_{\boldsymbol{k}}\hat{a}^{\dagger}_{\boldsymbol{k},l_2}\hat{a}_{\boldsymbol{k},l_3}\Bigg) \\
&+ \frac{1}{6}N_xN_yN_z\sum_{\boldsymbol{q}}\left(-n_{l_1,l_3}(-\boldsymbol{q})n_{l_2,l_4}(\boldsymbol{q}) - n_{l_1,l_4}(\boldsymbol{q})n_{l_2,l_3}(-\boldsymbol{q}) - x_{l_3,l_4}(\boldsymbol{q})x^{*}_{l_1,l_2}(\boldsymbol{q})\right),
\end{aligned}
$$

$$
\begin{aligned}
\hat{\mathcal{H}}^{\mathsf{D_{4h}}}_{int} \rightarrow{}& \frac{1}{2}\frac{1}{6}\sum_{\boldsymbol{k},\boldsymbol{k}'}\sum_{l}(u+w)\Bigg[2n_{l,l}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},l}\hat{a}_{\boldsymbol{k}',l} + 2n_{l,l}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}_{-\boldsymbol{k},l}\hat{a}^{\dagger}_{-\boldsymbol{k}',l} \\
&+ x^{*}_{l,l}(\boldsymbol{k}'-\boldsymbol{k})\hat{a}_{-\boldsymbol{k},l}\hat{a}_{\boldsymbol{k}',l} + x_{l,l}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},l}\hat{a}^{\dagger}_{-\boldsymbol{k}',l}\Bigg] \\
&- \frac{1}{2}\frac{1}{6}\sum_{\boldsymbol{k},\boldsymbol{k}'}\sum_{l}v\Bigg[2n_{l,\bar{l}}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},l}\hat{a}_{\boldsymbol{k}',\bar{l}} + 2n_{l,\bar{l}}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}_{-\boldsymbol{k},\bar{l}}\hat{a}^{\dagger}_{-\boldsymbol{k}',l} \\
&+ x^{*}_{l,l}(\boldsymbol{k}'-\boldsymbol{k})\hat{a}_{-\boldsymbol{k},\bar{l}}\hat{a}_{\boldsymbol{k}',\bar{l}} + x_{\bar{l},\bar{l}}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},l}\hat{a}^{\dagger}_{-\boldsymbol{k}',l}\Bigg] \\
&+ \frac{1}{2}\frac{1}{3}\sum_{\boldsymbol{k},\boldsymbol{k}'}(u+v-w)\Bigg[\sum_{l}\frac{1}{2}\left(n_{l,l}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},\bar{l}}\hat{a}_{\boldsymbol{k}',\bar{l}} + n_{l,l}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}_{-\boldsymbol{k},\bar{l}}\hat{a}^{\dagger}_{-\boldsymbol{k}',\bar{l}}\right) \\
&+ \sum_{l}\frac{1}{2}\left(n_{l,\bar{l}}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},\bar{l}}\hat{a}_{\boldsymbol{k}',l} + n_{l,\bar{l}}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}_{-\boldsymbol{k},l}\hat{a}^{\dagger}_{-\boldsymbol{k}',\bar{l}}\right) + x^{*}_{1,2}(\boldsymbol{k}'-\boldsymbol{k})\hat{a}_{-\boldsymbol{k},1}\hat{a}_{\boldsymbol{k}',2} \\
&+ \frac{1}{2}\left(x_{1,2}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},1}\hat{a}^{\dagger}_{-\boldsymbol{k}',2} + x_{1,2}(\boldsymbol{k}-\boldsymbol{k}')\hat{a}^{\dagger}_{\boldsymbol{k},2}\hat{a}^{\dagger}_{-\boldsymbol{k}',1}\right)\Bigg] \\
&- \left(\frac{(u+w)}{3} + \frac{(u+v-w)}{6}\right)\sum_{l}\sum_{\boldsymbol{k}}\hat{a}^{\dagger}_{\boldsymbol{k},l}\hat{a}_{\boldsymbol{k},l} - \frac{1}{2}\frac{1}{6}\sum_{\boldsymbol{k}}\sum_{l}(u+w)2n_{l,l}(0) \\
&- \frac{1}{2}\frac{1}{3}\sum_{l}\frac{1}{2}\sum_{\boldsymbol{k}}(u+v-w)\,n_{l,l}(0) + \frac{1}{2}\sum_{l}(u+w)\frac{1}{6}N_xN_yN_z\sum_{\boldsymbol{q}}\left(-2|n_{l,l}(\boldsymbol{q})|^2 - |x_{l,l}(\boldsymbol{q})|^2\right) \\
&- \frac{1}{2}\sum_{l}v\frac{1}{6}N_xN_yN_z\sum_{\boldsymbol{q}}\left(-2n^{*}_{\bar{l},l}(\boldsymbol{q})n_{l,\bar{l}}(\boldsymbol{q}) - x_{\bar{l},\bar{l}}(\boldsymbol{q})x^{*}_{l,l}(\boldsymbol{q})\right) \\
&+ (u+v-w)\,\frac{1}{6}N_xN_yN_z\sum_{\boldsymbol{q}}\left(-n^{*}_{1,1}(\boldsymbol{q})n_{2,2}(\boldsymbol{q}) - |n_{1,2}(\boldsymbol{q})|^2 - |x_{1,2}(\boldsymbol{q})|^2\right)
\end{aligned}
$$

Eventually, one obtains the mean–field Hamiltonian

$$\hat{\mathcal{H}}^{MF}_{D_{4h}} = \frac{1}{2}\left(\hat{\boldsymbol{a}}^\dagger, \hat{\boldsymbol{a}}\right) H_{BdG} \begin{pmatrix} \hat{\boldsymbol{a}} \\ \hat{\boldsymbol{a}}^\dagger \end{pmatrix} + \tilde{\mu}_0 \frac{1}{2} N - \frac{1}{4} N \frac{3u+v+w}{6} \sum_l n_{l,l}(0)$$
$$+ \frac{1}{6} N_x N_y N_z \sum_{\boldsymbol{q}} \left(-\frac{u+w-v}{4} \left| x_{1,1}(\boldsymbol{q}) + x_{2,2}(\boldsymbol{q}) \right|^2 - \frac{u+w+v}{4} \left| x_{1,1}(\boldsymbol{q}) - x_{2,2}(\boldsymbol{q}) \right|^2 - \frac{u+v-w}{4} |2x_{1,2}(\boldsymbol{q})|^2 \right)$$
$$+ \frac{1}{6} N_x N_y N_z \sum_{\boldsymbol{q}} \left(-\frac{3u+w+v}{4} \left| n_{1,1}(\boldsymbol{q}) + n_{2,2}(\boldsymbol{q}) \right|^2 - \frac{u+3w-v}{4} \left| n_{1,1}(\boldsymbol{q}) - n_{2,2}(\boldsymbol{q}) \right|^2 \right.$$
$$\left. - \frac{u-w-v}{4} \left| n_{1,2}(\boldsymbol{q}) + n_{2,1}(\boldsymbol{q}) \right|^2 - \frac{u+3v-w}{4} \left| n_{1,2}(\boldsymbol{q}) - n_{2,1}(\boldsymbol{q}) \right|^2 \right), \tag{1}$$

where we have introduced

$$\tilde{\mu}_0 = \mu_0 + \frac{(u+w)}{3} + \frac{(u+v-w)}{6} = \mu_0 + \frac{3u+v+w}{6}, \qquad \sum_{\boldsymbol{k}} 1 = \frac{1}{2} N = N_x N_y N_z,$$

and the Bogoliubov-deGennes Hamiltonian

$$H_{BdG} = \begin{pmatrix} M & \Delta \\ \Delta^\dagger & M^T \end{pmatrix},$$

with $M^\dagger = M$ and $\Delta^T = \Delta$. The basis vector reads

$$\hat{\boldsymbol{a}} = \begin{pmatrix} \hat{a}_{\boldsymbol{k}_1,1} \\ \hat{a}_{\boldsymbol{k}_1,2} \\ \hat{a}_{\boldsymbol{k}_2,1} \\ \hat{a}_{\boldsymbol{k}_2,2} \\ \dots \end{pmatrix}, \qquad \hat{\boldsymbol{a}}^\dagger = \begin{pmatrix} \hat{a}^\dagger_{-\boldsymbol{k}_1,1} \\ \hat{a}^\dagger_{-\boldsymbol{k}_1,2} \\ \hat{a}^\dagger_{-\boldsymbol{k}_2,1} \\ \hat{a}^\dagger_{-\boldsymbol{k}_2,2} \\ \dots \end{pmatrix}.$$

For the diagonalization, we introduce the new bosonic basis defined by

$$\left(\hat{\boldsymbol{a}}^\dagger, \hat{\boldsymbol{a}}\right) = \left(\hat{\boldsymbol{\alpha}}^\dagger, \hat{\boldsymbol{\alpha}}\right) T^\dagger, \qquad \begin{pmatrix} \hat{\boldsymbol{a}} \\ \hat{\boldsymbol{a}}^\dagger \end{pmatrix} = T \begin{pmatrix} \hat{\boldsymbol{\alpha}} \\ \hat{\boldsymbol{\alpha}}^\dagger \end{pmatrix}, \qquad T = \begin{pmatrix} U & V \\ V^* & U^* \end{pmatrix}$$
$$\begin{pmatrix} \hat{\boldsymbol{\alpha}} \\ \hat{\boldsymbol{\alpha}}^\dagger \end{pmatrix} = \Sigma_z T^\dagger \Sigma_z \begin{pmatrix} \hat{\boldsymbol{a}} \\ \hat{\boldsymbol{a}}^\dagger \end{pmatrix}, \qquad T^\dagger = \begin{pmatrix} U^\dagger & V^T \\ V^\dagger & U^T \end{pmatrix},$$

with the para-unitary matrix T. One notes that in order to satisfy bosonic commutation relations

$$\left[\hat{\alpha}_i, \hat{\alpha}_j\right] = \left(V^T U^* - U^\dagger V\right)_{ij} = 0 \tag{2}$$

$$\left[\hat{\alpha}^\dagger_i, \hat{\alpha}^\dagger_j\right] = \left(U^T V^* - V^\dagger U\right)_{ij} = 0, \tag{3}$$

$$\left[\hat{\alpha}_i, \hat{\alpha}^\dagger_j\right] = \left(U^\dagger U - V^T V^*\right)_{ij} = \delta_{ij} \tag{4}$$

the matrix T has to satisfy

$$T^{\dagger}\Sigma_z T = \Sigma_z \tag{5}$$

with $\Sigma_{x,z} = \sigma_{x,z} \otimes \mathbb{1}$. Then, the mean-field Hamiltonian becomes

$$\begin{aligned}
\hat{\mathcal{H}}^{MF} &= \frac{1}{2}\left(\hat{\boldsymbol{\alpha}}^{\dagger}, \hat{\boldsymbol{\alpha}}\right)\Sigma_z T^{-1}\underbrace{\Sigma_z H_{BdG}}_{=\tilde{H}_{BdG}} T\begin{pmatrix}\hat{\boldsymbol{\alpha}}\\ \hat{\boldsymbol{\alpha}}^{\dagger}\end{pmatrix} + \tilde{\mu}_0\frac{1}{2}N - \frac{1}{4}N\frac{3u+v+w}{6}\sum_l n_{l,l}(0)\\
&= \frac{1}{2}\left(\hat{\boldsymbol{\alpha}}^{\dagger}, \hat{\boldsymbol{\alpha}}\right)\Sigma_z \Lambda\begin{pmatrix}\hat{\boldsymbol{\alpha}}\\ \hat{\boldsymbol{\alpha}}^{\dagger}\end{pmatrix} + \tilde{\mu}_0\frac{1}{2}N - \frac{1}{4}N\frac{3u+v+w}{6}\sum_l n_{l,l}(0),
\end{aligned}$$

where $\Lambda = \mathrm{diag}\left(\Lambda_1, \Lambda_2, \Lambda_3, \dots\right)$ is a diagonal matrix. Now, we see that we actually have to diagonalize the matrix

$$\tilde{H}_{BdG} = \Sigma_z H_{BdG}$$

by means of the matrix T. The new Hamiltonian satisfies a pseudo-Hermiticity

$$\Sigma_z \tilde{H}^{\dagger}_{BdG}\Sigma_z = \tilde{H}_{BdG},$$

and it satisfies a particle-hole symmetry

$$\Sigma_x \tilde{H}^{*}_{BdG}\Sigma_x = -\tilde{H}_{BdG},$$

As a consequence of the latter, eigenstates come in pairs of

$$\left\{\omega_i, -\omega_i^*\right\} \quad \text{with} \quad \left\{\tilde{\boldsymbol{v}}^{(+)}_{i,\ell}, \tilde{\boldsymbol{v}}^{(-)}_{i,\ell}\right\} = \left\{\begin{pmatrix}\tilde{\boldsymbol{U}}_{i,\ell}\\ \tilde{\boldsymbol{V}}^*_{i,\ell}\end{pmatrix}, \begin{pmatrix}\tilde{\boldsymbol{V}}_{i,\ell}\\ \tilde{\boldsymbol{U}}^*_{i,\ell}\end{pmatrix}\right\},$$

where we introduce the index ℓ to account for degeneracies. Assuming that the above eigenvectors are normalized, i.e.

$$1 = \tilde{\boldsymbol{U}}^{\dagger}_{i,\ell}\tilde{\boldsymbol{U}}_{i,\ell} + \tilde{\boldsymbol{V}}^{T}_{i,\ell}\tilde{\boldsymbol{V}}^{*}_{i,\ell},$$

then, they have to be rescaled via

$$\left\{\begin{pmatrix}\boldsymbol{U}_{i,\ell}\\ \boldsymbol{V}^*_{i,\ell}\end{pmatrix}, \begin{pmatrix}\boldsymbol{V}_{i,\ell}\\ \boldsymbol{U}^*_{i,\ell}\end{pmatrix}\right\} = \frac{1}{\sqrt{|\tilde{\boldsymbol{U}}^{\dagger}_{i,\ell}\tilde{\boldsymbol{U}}_{i,\ell} - \tilde{\boldsymbol{V}}^{T}_{i,\ell}\tilde{\boldsymbol{V}}^{*}_{i,\ell}|}}\left\{\begin{pmatrix}\tilde{\boldsymbol{U}}_{i,\ell}\\ \tilde{\boldsymbol{V}}^*_{i,\ell}\end{pmatrix}, \begin{pmatrix}\tilde{\boldsymbol{V}}_{i,\ell}\\ \tilde{\boldsymbol{U}}^*_{i,\ell}\end{pmatrix}\right\},$$

in order for T to satisfy (5). This can be seen from the Schroedinger equations

$$\left[\hat{\alpha}_{i,\ell}, \hat{\alpha}_{j,\ell'}\right] = \left(\boldsymbol{w}^{(2)}_{i,\ell}\right)^{\dagger}\boldsymbol{w}^{(3)}_{j,\ell'} = 0 \tag{6}$$

$$\left[\hat{\alpha}^{\dagger}_{i,\ell}, \hat{\alpha}^{\dagger}_{j,\ell'}\right] = \boldsymbol{U}^{T}_{i,\ell}\boldsymbol{V}^{*}_{j,\ell'} - \boldsymbol{V}^{\dagger}_{i,\ell}\boldsymbol{U}_{j,\ell'} = 0, \tag{7}$$

$$\left[\hat{\alpha}_{i,\ell}, \hat{\alpha}^{\dagger}_{j,\ell'}\right] = \left(\boldsymbol{w}^{(2)}_{i,\ell}\right)^{\dagger}\boldsymbol{w}^{(1)}_{j,\ell'} = \delta_{ij}\delta_{\ell\ell'}, \tag{8}$$

where we have introduced

$$\boldsymbol{w}^{(1)}_{i,\ell} = \begin{pmatrix} \boldsymbol{U}_{i,\ell} \\ \boldsymbol{V}^*_{i,\ell} \end{pmatrix}, \qquad \boldsymbol{w}^{(2)}_{i,\ell} = \begin{pmatrix} \boldsymbol{U}_{i,\ell} \\ -\boldsymbol{V}^*_{i,\ell} \end{pmatrix} = \Sigma_z \boldsymbol{w}^{(1)}_{i,\ell}, \qquad \boldsymbol{w}^{(3)}_{i,\ell} = \begin{pmatrix} \boldsymbol{V}_{i,\ell} \\ \boldsymbol{U}^*_{i,\ell} \end{pmatrix} = \Sigma_x \mathcal{K} \boldsymbol{w}^{(1)}_{i,\ell},$$

with $i \in [1, N]$. It is clear that if the above conditions hold, then also equation (5) holds. As shown in the first chapter, the above relations hold automatically, except for degenerate subspaces. There, we have to make sure it holds

$$\left(\boldsymbol{w}^{(2)}_{i,\ell'}\right)^\dagger \boldsymbol{w}^{(1)}_{i,\ell} = \left(\boldsymbol{w}^{(1)}_{i,\ell'}\right)^\dagger \Sigma_z \boldsymbol{w}^{(1)}_{i,\ell} = \delta_{\ell\ell'}, \tag{9}$$

which can be taken care of as explained in the box in the first chapter.

Eventually, the diagonal matrix becomes

$$\begin{aligned} \Lambda &= \mathrm{diag}\left(\omega_1, \omega_2, \ldots, \omega_N, -\omega_1, -\omega_2, \ldots, -\omega_N\right), \\ \Sigma_z \Lambda &= \mathrm{diag}\left(\omega_1, \omega_2, \ldots, \omega_N, \omega_1, \omega_2, \ldots, \omega_N\right) = \begin{pmatrix} \tilde{\Lambda} & 0 \\ 0 & \tilde{\Lambda} \end{pmatrix} = \tilde{\Lambda} \otimes \mathbb{1}_2, \end{aligned}$$

where we have assumed $\omega_i^* = \omega_i$. Note that, due to the diagonalization the eigenenergies are functions of the chemical potential $\omega_i = \omega_i(\mu_0)$. Then, the Hamiltonian finally becomes

$$\begin{aligned} \hat{\mathcal{H}}^{MF} &= \frac{1}{2}\left(\hat{\boldsymbol{\alpha}}^\dagger, \hat{\boldsymbol{\alpha}}\right) \begin{pmatrix} \tilde{\Lambda} & 0 \\ 0 & \tilde{\Lambda} \end{pmatrix} \begin{pmatrix} \hat{\boldsymbol{\alpha}} \\ \hat{\boldsymbol{\alpha}}^\dagger \end{pmatrix} + \tilde{\mu}_0 \frac{1}{2} N - \frac{1}{4} N \frac{3u + v + w}{6} \sum_l n_{l,l}(0) \\ &= \frac{1}{2} \sum_{i=1}^{N} \omega_i(\mu_0) \left(\hat{\alpha}_i^\dagger \hat{\alpha}_i + \hat{\alpha}_i \hat{\alpha}_i^\dagger\right) - \frac{1}{2} N \left(-\tilde{\mu}_0 + \frac{3u + v + w}{12} \sum_l n_{l,l}(0)\right) \\ &= \sum_{i=1}^{N} \omega_i(\mu_0) \left(\hat{\alpha}_i^\dagger \hat{\alpha}_i + \frac{1}{2}\right) - \frac{1}{2} N R_0, \end{aligned}$$

Using the inverse relation

$$\begin{aligned} \begin{pmatrix} \hat{\boldsymbol{a}} \\ \hat{\boldsymbol{a}}^\dagger \end{pmatrix} = T \begin{pmatrix} \hat{\boldsymbol{\alpha}} \\ \hat{\boldsymbol{\alpha}}^\dagger \end{pmatrix} &= \begin{pmatrix} U \hat{\boldsymbol{\alpha}} + V \hat{\boldsymbol{\alpha}}^\dagger \\ V^* \hat{\boldsymbol{\alpha}} + U^* \hat{\boldsymbol{\alpha}}^\dagger \end{pmatrix}, \\ \hat{a}_i &= U_{ii'} \hat{\alpha}_{i'} + V_{ii'} \hat{\alpha}^\dagger_{i'}, \\ \hat{a}^\dagger_i &= V^*_{ii'} \hat{\alpha}_{i'} + U^*_{ii'} \hat{\alpha}^\dagger_{i'}, \end{aligned}$$

$$
\begin{aligned}
\langle\hat{\mathcal{H}}^{MF}\rangle &= \sum_{i=1}^{N}\omega_i(\mu_0)\left(n_B(\omega_i(\mu_0))+\frac{1}{2}\right)+\tilde{\mu}_0\frac{1}{2}N-\frac{1}{4}N\frac{3u+v+w}{6}\sum_l n_{l,l}(0), \\
Z_G &= e^{-\left(\tilde{\mu}_0\frac{1}{2}N-\frac{1}{4}N\frac{3u+v+w}{6}\sum_l n_{l,l}(0)\right)/T}\prod_{i=1}^{N}\frac{e^{-\frac{1}{2}\omega_i(\mu_0)/T}}{1-e^{-\omega_i(\mu_0)/T}},
\end{aligned}
\tag{10}
$$

$$
\begin{aligned}
\Omega &= -T\log Z_G \\
&= \tilde{\mu}_0\frac{1}{2}N-\frac{1}{4}N\frac{3u+v+w}{6}\sum_l n_{l,l}(0)+\frac{1}{2}\sum_{i=1}^{N}\omega_i(\mu_0)+T\sum_{i=1}^{N}\log\left(1-e^{-\omega_i(\mu_0)/T}\right) \\
&= \tilde{\mu}_0\frac{1}{2}N-\frac{1}{4}N\frac{3u+v+w}{6}\sum_l n_{l,l}(0)-\sum_{i=1}^{N}\left(\frac{1}{2}\omega_i(\mu_0)+T\log n_B(\omega_i(\mu_0))\right), \\
F &= \Omega+\mu_0\bar{N},
\end{aligned}
\tag{11}
$$

$$
\begin{aligned}
\bar{N} &= -\frac{\partial\Omega}{\partial\mu_0}\Big|_{V,T} \\
&= -\frac{1}{2}N+\sum_{i=1}^{N}\left(\frac{1}{2}-\frac{e^{\beta\omega_i(\mu_0)}}{e^{\beta\omega_i(\mu_0)}-1}\right)\frac{\partial\omega_i(\mu_0)}{\partial\mu_0}\Big|_{V,T}, \\
&= \sum_{i=1}^{N}\left(\frac{1}{e^{\beta\omega_i(\mu_0)}-1}\left(U^\dagger U\right)_{ii}+\frac{e^{\beta\omega_i(\mu_0)}}{e^{\beta\omega_i(\mu_0)}-1}\left(V^TV^*\right)_{ii}\right) \\
&= \sum_{i=1}^{N}\left(\frac{1}{e^{\beta\omega_i(\mu_0)}-1}+\frac{e^{\beta\omega_i(\mu_0)}+1}{e^{\beta\omega_i(\mu_0)}-1}\left(V^TV^*\right)_{ii}\right) \\
&= \mathrm{tr}\left(\hat{n}_B\left(U^\dagger U\right)+(1+\hat{n}_B)\left(V^TV^*\right)\right), \\
\bar{N} &= \sum_{i=1}^{N}\langle\hat{a}_i^\dagger\hat{a}_i\rangle=\mathrm{tr}\left(V^TV^*+\left(V^TV^*+U^TU^*\right)\hat{n}_B\right)
\end{aligned}
\tag{12}
$$

Using

$$
\begin{aligned}
\Lambda &= T^{-1}\Sigma_z H_{BdG} T = \Sigma_z T^{\dagger}\left(H^0_{BdG} - \tilde{\mu}_0\{1\}\right) T \\
&= \begin{pmatrix} U^{\dagger} & V^T \\ -V^{\dagger} & -U^T \end{pmatrix}\begin{pmatrix} M & \Delta \\ \Delta^{\dagger} & M^T \end{pmatrix}\begin{pmatrix} U & V \\ V^* & U^* \end{pmatrix} \\
&= \begin{pmatrix} U^{\dagger}\left(MU+\Delta V^*\right)+V^T\left(\Delta^{\dagger}U+M^T V^*\right) & U^{\dagger}\left(MV+\Delta U^*\right)+V^T\left(\Delta^{\dagger}V+M^T U^*\right) \\ -V^{\dagger}\left(MU+\Delta V^*\right)-U^T\left(\Delta^{\dagger}U+M^T V^*\right) & -V^{\dagger}\left(MV+\Delta U^*\right)-U^T\left(\Delta^{\dagger}V+M^T U^*\right) \end{pmatrix}, \\
\omega_i(\mu_0) &= \left(U^{\dagger}MU + V^T M^T V^* + U^{\dagger}\Delta V^* + V^T\Delta^{\dagger}U\right)_{ii} \\
&= \left(U^{\dagger}M_0 U + V^T M_0^T V^* - \tilde{\mu}_0\left(U^{\dagger}U + V^T V^*\right) + U^{\dagger}\Delta V^* + V^T\Delta^{\dagger}U\right)_{ii}, \\
\omega_i(\mu_0) &= \left(V^{\dagger}MV + U^T M^T U^* + V^{\dagger}\Delta U^* + U^T\Delta^{\dagger}V\right)_{ii} \\
M &= M_0 - \tilde{\mu}_0\{1\}, \\
\frac{\partial\omega_i(\mu_0)}{\partial\mu_0}\Big|_{V,T}\Big|_{U,V} &= -\left(U^{\dagger}U + V^T V^*\right)_{ii}
\end{aligned}
$$

and the relations

$$
\begin{aligned}
\langle\hat{\alpha}_i^{\dagger}\hat{\alpha}_{i'}\rangle &= \mathrm{tr}\left(\hat{\alpha}_i^{\dagger}\hat{\alpha}_{i'}\frac{1}{Z_G}e^{-\beta\hat{\mathcal{H}}^{MF}}\right) = n_B(\omega_i(\mu_0))\delta_{i,i'}, \\
\langle\hat{\alpha}_i\hat{\alpha}_{i'}\rangle &= \langle\hat{\alpha}_i^{\dagger}\hat{\alpha}_{i'}^{\dagger}\rangle = 0,
\end{aligned}
$$

with the Bose function

$$
n_B(E) = \frac{1}{e^{\beta E}-1}, \qquad\qquad 1+n_B(E) = \frac{e^{\beta E}}{e^{\beta E}-1},
$$

we can express the desired expectation values as

$$
\begin{aligned}
\langle\hat{a}_i^{\dagger}\hat{a}_j\rangle &= \langle\left(V^*_{ii'}\hat{\alpha}_{i'} + U^*_{ii'}\hat{\alpha}^{\dagger}_{i'}\right)\left(U_{jj'}\hat{\alpha}_{j'} + V_{jj'}\hat{\alpha}^{\dagger}_{j'}\right)\rangle \\
&= V^*_{ii'}V_{jj'}\langle\hat{\alpha}_{i'}\hat{\alpha}^{\dagger}_{j'}\rangle + U^*_{ii'}U_{jj'}\langle\hat{\alpha}^{\dagger}_{i'}\hat{\alpha}_{j'}\rangle \\
&= V^*_{ii'}V^T_{i'j} + V^*_{ii'}n_B(\omega_{i'})V^T_{i'j} + U^*_{ii'}n_B(\omega_{i'})U^T_{i'j} \\
&= V^*_{ii'}\left(1+n_B(\omega_{i'})\right)V^T_{i'j} + U^*_{ii'}n_B(\omega_{i'})U^T_{i'j} \\
&= \left(V^*\left(\mathbb{1}+\hat{n}_B\right)V^T + U^*\hat{n}_B U^T\right)_{ij}, \\
\hat{n}_B &= \mathrm{diag}\left(n_B(\omega_1), n_B(\omega_2), \ldots\right),
\end{aligned}
$$

and

$$\begin{aligned}
\langle \hat{a}_i \hat{a}_j \rangle &= \langle \left(U_{ii'} \hat{\alpha}_{i'} + V_{ii'} \hat{\alpha}^\dagger_{i'} \right) \left(U_{jj'} \hat{\alpha}_{j'} + V_{jj'} \hat{\alpha}^\dagger_{j'} \right) \rangle \\
&= U_{ii'} \left(1 + n_B(\omega_{i'})\right) V^T_{i'j} + V_{ii'} n_B(\omega_{i'}) U^T_{i'j} \\
&= \left(U \left(\mathbb{1} + \hat{n}_B\right) V^T + V \hat{n}_B U^T \right)_{ij} \\
\langle \hat{a}^\dagger_i \hat{a}^\dagger_j \rangle &= \langle \left(V^*_{ii'} \hat{\alpha}_{i'} + U^*_{ii'} \hat{\alpha}^\dagger_{i'} \right) \left(V^*_{jj'} \hat{\alpha}_{j'} + U^*_{jj'} \hat{\alpha}^\dagger_{j'} \right) \rangle \\
&= V^*_{ii'} \left(1 + n_B(\omega_{i'})\right) U^\dagger_{i'j} + U^*_{ii'} n_B(\omega_{i'}) V^\dagger_{i'j} \\
&= \left(V^* \left(\mathbb{1} + \hat{n}_B\right) U^\dagger \right)_{ij} + \left(U^* \hat{n}_B V^\dagger \right)_{ij} \\
&= \left(V^* \left(\mathbb{1} + \hat{n}_B\right) U^\dagger + U^* \hat{n}_B V^\dagger \right)_{ij},
\end{aligned}$$

A. Check for automatically satisfied $T_{\boldsymbol{k}}$ conditions

$$\boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}} = \begin{pmatrix} U_{i,\ell,\boldsymbol{k}} \\ V^*_{i,\ell,-\boldsymbol{k}} \end{pmatrix}, \qquad \boldsymbol{w}^{(2)}_{i,\ell,\boldsymbol{k}} = \begin{pmatrix} U_{i,\ell,\boldsymbol{k}} \\ -V^*_{i,\ell,-\boldsymbol{k}} \end{pmatrix} = \Sigma_z \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}}, \qquad \boldsymbol{w}^{(3)}_{i,\ell,\boldsymbol{k}} = \begin{pmatrix} \boldsymbol{V}_{i,\ell,-\boldsymbol{k}} \\ \boldsymbol{U}^*_{i,\ell,\boldsymbol{k}} \end{pmatrix} = \Sigma_x \mathcal{K} \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}}.$$

It is clear that if the above conditions hold, then also equation (**??**) holds. Now, let us write the Schroedinger equation for one eigenvector in the different ways

$$\tilde{H}_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}} = \omega_{i,\boldsymbol{k}} \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}}. \tag{13}$$

where $i \in [1, N]$. The Hamiltonian has the properties

$$\tilde{H}_{BdG}(-\boldsymbol{k}) = \tilde{H}_{BdG}(\boldsymbol{k}), \tag{14}$$

$$\Sigma_x \mathcal{K} \tilde{H}_{BdG}(\boldsymbol{k}) \mathcal{K} \Sigma_x = -\tilde{H}_{BdG}(\boldsymbol{k}), \tag{15}$$

$$\Sigma_z \tilde{H}_{BdG}(\boldsymbol{k}) \Sigma_z = \tilde{H}^\dagger_{BdG}(\boldsymbol{k}). \tag{16}$$

Relation (14) directly says that it has to hold $\omega_{i,-\boldsymbol{k}} = \omega_{i,\boldsymbol{k}}$ and hence

$$\tilde{H}_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(1)}_{i,\ell,-\boldsymbol{k}} = \omega_{i,\boldsymbol{k}} \boldsymbol{w}^{(1)}_{i,\ell,-\boldsymbol{k}}, \tag{17}$$

which makes $\boldsymbol{w}^{(1)}_{i,\ell,\pm\boldsymbol{k}}$ either the same state, or degenerate states. Relations (15) and (16) provide the further equations

$$\begin{aligned}
\tilde{H}_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(3)}_{i,\ell,\boldsymbol{k}} &= -\omega^*_{i,\boldsymbol{k}} \boldsymbol{w}^{(3)}_{i,\ell,\boldsymbol{k}}, \\
\tilde{H}^\dagger_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(2)}_{i,\ell,\boldsymbol{k}} &= \omega_{i,\boldsymbol{k}} \boldsymbol{w}^{(2)}_{i,\ell,\boldsymbol{k}}.
\end{aligned}$$

In the following we assume that it holds $\omega^*_{i,\boldsymbol{k}} \neq -\omega_{i,\boldsymbol{k}}$, i.e. $\omega_{i,\boldsymbol{k}} \notin \mathrm{i}\mathbb{R}$. [Otherwise, it would hold $\left(\boldsymbol{w}^{(1)}_{i,\boldsymbol{k}}\right)^\dagger \Sigma_z \boldsymbol{w}^{(1)}_{i,\boldsymbol{k}} = 0$.] From the definition of $\boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}}$ we find

$$\omega_i \left(\boldsymbol{w}^{(2)}_{i,\ell'}\right)^\dagger \boldsymbol{w}^{(1)}_{i,\ell} = \omega_i \left(\boldsymbol{w}^{(1)}_{i,\ell'}\right)^\dagger \Sigma_z \boldsymbol{w}^{(1)}_{i,\ell} = \left(\boldsymbol{w}^{(2)}_{i,\ell'}\right)^\dagger \tilde{H}_{BdG} \boldsymbol{w}^{(1)}_{i,\ell} = \left(\boldsymbol{w}^{(1)}_{i,\ell'}\right)^\dagger H_{BdG} \boldsymbol{w}^{(1)}_{i,\ell},$$
$$\omega_i^* \left(\boldsymbol{w}^{(1)}_{i,\ell}\right)^\dagger \Sigma_z \boldsymbol{w}^{(1)}_{i,\ell'} = \left(\boldsymbol{w}^{(1)}_{i,\ell}\right)^\dagger H_{BdG} \boldsymbol{w}^{(1)}_{i,\ell'}$$
$$\omega_i^* = \omega_i,$$

and hence $\omega_i \in \mathbb{R}$. In the following, we show that it holds

$$0 = \left[\hat{\alpha}_{\boldsymbol{k},i}, \hat{\alpha}_{\boldsymbol{k}',j}\right] = \delta_{\boldsymbol{k},-\boldsymbol{k}'} \left(\left(V^T_{-\boldsymbol{k}}\right)_{ii'} (U^*_{-\boldsymbol{k}})_{i'j} - \left(U^\dagger_{\boldsymbol{k}}\right)_{ii'} (V_{\boldsymbol{k}})_{i'j}\right) = \left(\boldsymbol{w}^{(2)}_{i,\ell,\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(3)}_{j,\ell',-\boldsymbol{k}} \tag{18}$$
$$0 = \left[\hat{\alpha}^\dagger_{\boldsymbol{k},i}, \hat{\alpha}^\dagger_{\boldsymbol{k}',j}\right] = \delta_{\boldsymbol{k},-\boldsymbol{k}'} \left(-\left(V^\dagger_{-\boldsymbol{k}}\right)_{ii'} (U_{-\boldsymbol{k}})_{i'j} + \left(U^T_{\boldsymbol{k}}\right)_{ii'} (V^*_{\boldsymbol{k}})_{i'j}\right) = \left(\boldsymbol{w}^{(3)}_{i,\ell,\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(2)}_{j,\ell',-\boldsymbol{k}} \tag{19}$$
$$\delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{ij}\delta_{\ell,\ell'} = \left[\hat{\alpha}_{\boldsymbol{k},i}, \hat{\alpha}^\dagger_{\boldsymbol{k}',j}\right] = \delta_{\boldsymbol{k},\boldsymbol{k}'} \left(\left(U^\dagger_{\boldsymbol{k}}\right)_{ii'} (U_{\boldsymbol{k}})_{i'j} - \left(V^T_{-\boldsymbol{k}}\right)_{ii'} (V^*_{-\boldsymbol{k}})_{i'j}\right) = \left(\boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(2)}_{j,\ell',\boldsymbol{k}} \tag{20}$$

which fulfills the commutation requirements (**??**)-(**??**). For this, we employ the matrix elements

$$\begin{aligned}
&\left(\boldsymbol{w}^{(2)}_{i',\ell',\boldsymbol{k}}\right)^\dagger \tilde{H}_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}} = \omega_{i,\boldsymbol{k}} \left(\boldsymbol{w}^{(2)}_{i',\ell',\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}},\\
&\left(\boldsymbol{w}^{(1)}_{j',\ell',\boldsymbol{k}}\right)^\dagger \tilde{H}^\dagger_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(2)}_{j,\ell,\boldsymbol{k}} = \omega_{j,\boldsymbol{k}} \left(\boldsymbol{w}^{(1)}_{j',\ell',\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(2)}_{j,\ell,\boldsymbol{k}} \qquad \rightarrow \left(\boldsymbol{w}^{(2)}_{j,\ell,\boldsymbol{k}}\right)^\dagger \tilde{H}_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(1)}_{j',\ell',\boldsymbol{k}} = \omega^*_{j,\boldsymbol{k}} \left(\boldsymbol{w}^{(2)}_{j,\ell,\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(1)}_{j',\ell',\boldsymbol{k}}\\
\rightarrow &\left(\boldsymbol{w}^{(2)}_{i',\ell',\boldsymbol{k}}\right)^\dagger \tilde{H}_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}} = \omega^*_{i',\boldsymbol{k}} \left(\boldsymbol{w}^{(2)}_{i',\ell',\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}},\\
&\left(\boldsymbol{w}^{(3)}_{j',\ell',\boldsymbol{k}}\right)^\dagger \tilde{H}^\dagger_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(2)}_{j,\ell,-\boldsymbol{k}} = \omega_{j,\boldsymbol{k}} \left(\boldsymbol{w}^{(3)}_{j',\ell',\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(2)}_{j,\ell,-\boldsymbol{k}} \quad \rightarrow \left(\boldsymbol{w}^{(2)}_{j,\ell,-\boldsymbol{k}}\right)^\dagger \tilde{H}_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(3)}_{j',\ell',\boldsymbol{k}} = \omega^*_{j,\boldsymbol{k}} \left(\boldsymbol{w}^{(2)}_{j,\ell,-\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(3)}_{j',\ell',\boldsymbol{k}}\\
\rightarrow &\left(\boldsymbol{w}^{(2)}_{i',\ell',-\boldsymbol{k}}\right)^\dagger \tilde{H}_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(3)}_{i,\ell,\boldsymbol{k}} = \omega^*_{i',\boldsymbol{k}} \left(\boldsymbol{w}^{(2)}_{i',\ell',-\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(3)}_{i,\ell,\boldsymbol{k}},\\
&\left(\boldsymbol{w}^{(2)}_{i',\ell',-\boldsymbol{k}}\right)^\dagger \tilde{H}_{BdG}(\boldsymbol{k}) \boldsymbol{w}^{(3)}_{i,\ell,\boldsymbol{k}} = -\omega^*_{i,\boldsymbol{k}} \left(\boldsymbol{w}^{(2)}_{i',\ell',-\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(3)}_{i,\ell,\boldsymbol{k}}
\end{aligned}$$

Subtracting the first two leads to

$$0 = \left(\omega_{i,\boldsymbol{k}} - \omega^*_{j,\boldsymbol{k}}\right) \left(\boldsymbol{w}^{(2)}_{j,\ell',\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}}.$$

Thus, we see for $i = j$ that it has to hold

$$\omega_{i,\boldsymbol{k}} = \omega^*_{i,\boldsymbol{k}},$$

Note that

$$\left(\boldsymbol{w}^{(2)}_{i,\ell,\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}} = \frac{\tilde{\boldsymbol{U}}^\dagger_{i,\ell,\boldsymbol{k}} \tilde{\boldsymbol{U}}_{i,\ell,\boldsymbol{k}} - \tilde{\boldsymbol{V}}^T_{i,\ell,-\boldsymbol{k}} \tilde{\boldsymbol{V}}^*_{i,\ell,-\boldsymbol{k}}}{|\tilde{\boldsymbol{U}}^\dagger_{i,\ell,\boldsymbol{k}} \tilde{\boldsymbol{U}}_{i,\ell,\boldsymbol{k}} - \tilde{\boldsymbol{V}}^T_{i,\ell,-\boldsymbol{k}} \tilde{\boldsymbol{V}}^*_{i,\ell,-\boldsymbol{k}}|} = 1.$$

For $i \neq j$, it has to hold

$$\left(\boldsymbol{w}^{(2)}_{j,\ell',\boldsymbol{k}}\right)^\dagger \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}} = 0,$$

and condition (20) would be satisfied if there were no degeneracies. However, for $\ell > 1$ there is no symmetry relation that guarantees

$$\left(\boldsymbol{w}^{(2)}_{i,\ell',\boldsymbol{k}}\right)^{\dagger} \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}} = \left(\boldsymbol{w}^{(1)}_{i,\ell',\boldsymbol{k}}\right)^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,\ell,\boldsymbol{k}} = \delta_{\ell\ell'}. \tag{21}$$

The extra condition (21) within a degenerate subspace has to be satisfied by hand. Subtraction of the third and fourth equation leads to

$$0 = \left(\omega^*_{j,\boldsymbol{k}} + \omega^*_{i,\boldsymbol{k}}\right) \left(\boldsymbol{w}^{(2)}_{j,\ell',-\boldsymbol{k}}\right)^{\dagger} \boldsymbol{w}^{(3)}_{i,\ell,\boldsymbol{k}},$$

and since for $i, j \in [1, N]$ [only half of the space] it should hold $\omega^*_{j,\boldsymbol{k}} + \omega^*_{i,\boldsymbol{k}} \neq 0$, the condition (18) is readily satisfied—even for the degenerate subspace. Eventually, we take

$$T_{\boldsymbol{k}} = \begin{pmatrix} U_{\boldsymbol{k}} & V_{\boldsymbol{k}} \\ V^*_{-\boldsymbol{k}} & U^*_{-\boldsymbol{k}} \end{pmatrix}, \qquad T_{-\boldsymbol{k}} = \begin{pmatrix} U_{-\boldsymbol{k}} & V_{-\boldsymbol{k}} \\ V^*_{\boldsymbol{k}} & U^*_{\boldsymbol{k}} \end{pmatrix},$$

for the pairs $\pm\boldsymbol{k}$. It is also to be expected that it holds $U_{-\boldsymbol{k}} = U_{\boldsymbol{k}}$ and $V_{-\boldsymbol{k}} = V_{\boldsymbol{k}}$.

B. Diagonalization of the degenerate subspace

The set of degenerate eigenvectors $\{\boldsymbol{w}^{(1)}_{i,1}, \ldots, \boldsymbol{w}^{(1)}_{i,\ell_{\max}}\}$ has to satisfy the condition (21). To this end, we apply a Gram-Schmidt type orthogonalization process where we construct new vectors $\{\tilde{\boldsymbol{w}}^{(1)}_{i,1}, \ldots, \tilde{\boldsymbol{w}}^{(1)}_{i,\ell_{\max}}\}$ that satisfy

$$\left(\tilde{\boldsymbol{w}}^{(1)}_{i,\ell'}\right)^{\dagger} \Sigma_z \tilde{\boldsymbol{w}}^{(1)}_{i,\ell} = \delta_{\ell\ell'}.$$

The first few vectors read

$$\tilde{\boldsymbol{w}}^{(1)}_{i,1} = \rho_1 \boldsymbol{w}^{(1)}_{i,1}, \qquad \rho_1 = \frac{1}{\sqrt{(\boldsymbol{w}^{(1)}_{i,1})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,1}}},$$

$$\tilde{\boldsymbol{w}}^{(1)}_{i,2} = \rho_2 \left(\boldsymbol{w}^{(1)}_{i,2} - \left((\tilde{\boldsymbol{w}}^{(1)}_{i,1})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,2}\right) \tilde{\boldsymbol{w}}^{(1)}_{i,1}\right), \qquad \rho_2 = \frac{1}{\sqrt{(\boldsymbol{w}^{(1)}_{i,2})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,2} - |(\tilde{\boldsymbol{w}}^{(1)}_{i,1})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,2}|^2}},$$

$$\tilde{\boldsymbol{w}}^{(1)}_{i,3} = \rho_3 \left(\boldsymbol{w}^{(1)}_{i,3} - \left((\tilde{\boldsymbol{w}}^{(1)}_{i,1})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,3}\right) \tilde{\boldsymbol{w}}^{(1)}_{i,1} - \left((\tilde{\boldsymbol{w}}^{(1)}_{i,2})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,3}\right) \tilde{\boldsymbol{w}}^{(1)}_{i,2}\right),$$
$$\rho_3 = \frac{1}{\sqrt{(\boldsymbol{w}^{(1)}_{i,3})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,3} - |(\tilde{\boldsymbol{w}}^{(1)}_{i,1})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,3}|^2 - |(\tilde{\boldsymbol{w}}^{(1)}_{i,2})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,3}|^2}}$$

and thus, in the compact form, we construct

$$\tilde{\boldsymbol{w}}^{(1)}_{i,\ell} = \rho_\ell \left(\boldsymbol{w}^{(1)}_{i,l} - \sum_{\ell'=1}^{\ell-1} \left((\tilde{\boldsymbol{w}}^{(1)}_{i,\ell'})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,\ell}\right) \tilde{\boldsymbol{w}}^{(1)}_{i,\ell'}\right), \qquad \rho_\ell = \frac{1}{\sqrt{(\boldsymbol{w}^{(1)}_{i,\ell})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,\ell} - \sum_{\ell'=1}^{\ell-1} |(\tilde{\boldsymbol{w}}^{(1)}_{i,\ell'})^{\dagger} \Sigma_z \boldsymbol{w}^{(1)}_{i,\ell}|^2}},$$