Supplementary notes on:

Exponential suppression of the topological gap in self-consistent intrinsic Majorana nanowires

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The full article is accessible in https://arxiv.org/abs/2412.15174. First part Hartree-Fock-Bogoliubov mean-field theory.

Part I
Hartree-Fock-Bogoliubov mean-field theory

I. HAMILTONIAN DESCRIPTION

Take an interacting many-body system of electrons described by the Hamiltonian

$$\begin{aligned} H &= H_0 + H_{\text{int}} \\ &= \sum_{\boldsymbol{ij}} c^\dagger_{\boldsymbol{i}} H_0^{\boldsymbol{ij}} c_{\boldsymbol{j}} + \frac{1}{2}\sum_{\boldsymbol{ij}}\sum_{\boldsymbol{i'j'}} c^\dagger_{\boldsymbol{i}} c_{\boldsymbol{i'}} V^{\boldsymbol{ij}}_{\boldsymbol{j'i'}} c^\dagger_{\boldsymbol{j}} c_{\boldsymbol{j'}} \end{aligned} \tag{1}$$

with $c^\dagger(c)$ fermionic creation (annihilation) operators and

$$\boldsymbol{i} \equiv (i, s_i) \tag{2}$$

composite degrees of freedom of purely spacial indices i and an additional orbital index at each site s_i such as spin. It follows directly from the composite notation that $\sum_{\boldsymbol{i}} = \sum_{s_i}\sum_i$ and $\delta_{\boldsymbol{ij}} = \delta_{ij}\delta_{s_i s_j}$.

A. Wannier spinless potential

Let us consider ultra-localized/Wannier orbitals such that the interaction tensor can approximately behave as

$$V^{\boldsymbol{ij}}_{\boldsymbol{j'i'}} \approx v^{\boldsymbol{ij}} \delta_{\boldsymbol{ii'}}\delta_{\boldsymbol{jj'}} \tag{3}$$

mediated by a spinless electrostatic scalar potential

$$v^{\boldsymbol{ij}} \to v^{ij} = v(\vec{r}_i - \vec{r}_j), \text{ with } v^{ij} = v^{ji}. \tag{4}$$

It follows that

$$\begin{aligned} H_{\text{int}} &= \frac{1}{2}\sum_{\boldsymbol{ij}}\sum_{\boldsymbol{i'j'}} c^\dagger_{\boldsymbol{i}} c_{\boldsymbol{i'}} \left(v^{\boldsymbol{ij}}\delta_{\boldsymbol{ii'}}\delta_{\boldsymbol{jj'}}\right) c^\dagger_{\boldsymbol{j}} c_{\boldsymbol{j'}} \\ &= \frac{1}{2}\sum_{\boldsymbol{ij}} c^\dagger_{\boldsymbol{i}} c_{\boldsymbol{i}} v^{ij} c^\dagger_{\boldsymbol{j}} c_{\boldsymbol{j}} \end{aligned} \tag{5}$$

A perturbation theory treatment of the interaction based on path integrals starts by casting the Hamiltonian into its normal-ordered form. Given the equal-time fermionic anti-commutator properties,

$$\{c_i, c_j^\dagger\} = c_i c_j^\dagger + c_j^\dagger c_i \tag{6}$$

$$\{c_i, c_j^\dagger\} = \{c_j^\dagger, c_i\} = \delta_{ij} \tag{7}$$

$$\{c_i, c_j\} = \{c_j^\dagger, c_i^\dagger\} = 0, \tag{8}$$

one obtains

$$\begin{aligned} H_{\text{int}} =& \frac{1}{2}\sum_{\boldsymbol{ij}} c^\dagger_{\boldsymbol{i}} c_{\boldsymbol{i}} v^{ij} c^\dagger_{\boldsymbol{j}} c_{\boldsymbol{j}} \\ =& \frac{1}{2}\sum_{\boldsymbol{ij}} c^\dagger_{\boldsymbol{i}} \left(\delta_{\boldsymbol{ij}} - c^\dagger_{\boldsymbol{j}} c_{\boldsymbol{i}}\right) c_{\boldsymbol{j}} v^{ij} \\ =& \frac{1}{2} c^\dagger_{\boldsymbol{i}} c_{\boldsymbol{i}} v^{ii} - \frac{1}{2}\sum_{\boldsymbol{ij}} c^\dagger_{\boldsymbol{i}} c^\dagger_{\boldsymbol{j}} v^{ij} c_{\boldsymbol{i}} c_{\boldsymbol{j}} \end{aligned} \tag{9}$$

See that from the normal ordering of H_{int} a non-physical spurious self-interaction term $1/2 c^\dagger_{\boldsymbol{i}} c_{\boldsymbol{i}} v^{ii}$ reveals itself explicitly, which should not take part since single electrons cannot interact with themselves. This term can be removed preemptively by incorporating it in Eq.(1) instead with a negative sign,

$$H_{\text{int}} - = \frac{1}{2}\sum_{\boldsymbol{i}} c^\dagger_{\boldsymbol{i}} c_{\boldsymbol{i}} v^{ii} \tag{10}$$

Within the scope of this approximation the normal-ordered Hamiltonians takes the form

$$H = \sum_{\boldsymbol{ij}} c^\dagger_{\boldsymbol{i}} H_0^{\boldsymbol{ij}} c_{\boldsymbol{j}} + \frac{1}{2}\sum_{\boldsymbol{ij}} c^\dagger_{\boldsymbol{i}} c^\dagger_{\boldsymbol{j}} v^{ij} c_{\boldsymbol{j}} c_{\boldsymbol{i}} \tag{11}$$

II. MEAN-FIELD HARTREE-FOCK-BOGOLIUBOV DECOUPLING

We wish to derive from Eq.(11) the explicit form of the Hartree/electrostatic Σ_H, Fock/exchange Σ_F and Bogoliubov/pairing Σ_B self-energies between spatial sites i and j, being matrices over orbital space. For this, one must Hartree-Fock-Bogoliubov decouple the Hamiltonian in Eq.(11) such that it could be expressed as:

$$H \approx H_0 + H^H_{\text{int}} + H^F_{\text{int}} + H^B_{\text{int}} \tag{12}$$
$$= \sum_{\boldsymbol{ij}} \left[c^\dagger_{\boldsymbol{i}} \left(H^{\boldsymbol{ij}}_0 + \Sigma^{\boldsymbol{ij}}_H + \Sigma^{\boldsymbol{ij}}_F \right) c_{\boldsymbol{j}} + \frac{1}{2} \left(c^\dagger_{\boldsymbol{i}} \Sigma^{\boldsymbol{ij}}_B c^\dagger_{\boldsymbol{j}} + h.c \right) \right].$$

In particular, within a Nambu-spinor representation, which we will be presenting next, we should be able to make this Hamiltonian the form

$$\check{H} = \frac{1}{2} \sum_{\boldsymbol{ij}} \check{c}_{\boldsymbol{i}} \left(\check{H}^{\boldsymbol{ij}}_0 + \check{\Sigma}^{\boldsymbol{ij}} \right) \check{c}_{\boldsymbol{j}}, \tag{13}$$

having an inherent Bogoliubov-de-Gennes (BdG) symmetry.

A. Nambu representation

For this derivation we focus on the system's reduced density matrix (rDM) equation of motion (EoM). In normal systems, i.e non-superconducting systems, the rDM defined as $\rho_{ee} = \langle c^\dagger_j c_i \rangle$ is sufficient, however, if one wishes to study superconducting systems, one must also account for the anomalous/pairing terms. For this, we introduce Nambu-spinors representation with doubling of degrees of freedom so that electron e, hole h become additional quantum numbers,

$$\check{c}^\dagger_i = \begin{pmatrix} c^\dagger_i & c_i \end{pmatrix} \text{ and } \check{c}_i = \begin{pmatrix} c_i \\ c^\dagger_i \end{pmatrix} \tag{14}$$

The corresponding Nambu rDM, can then be written as the direct/tensor product of this Nambu-spinors for each of the e, h combinations

$$\check{\rho}_{ij} = \langle \check{c}^\dagger_j \otimes \check{c}_i \rangle \tag{15}$$
$$= \begin{pmatrix} \langle c^\dagger_j c_i \rangle & \langle c_j c_i \rangle \\ \langle c^\dagger_j c^\dagger_i \rangle & \langle c_j c^\dagger_i \rangle \end{pmatrix} \equiv \begin{pmatrix} \rho^{ij}_{ee} & \rho^{ij}_{eh} \\ \rho^{ij}_{he} & \rho^{ij}_{hh} \end{pmatrix}$$

Directly from the equal-time fermionic anti-commutator properties in Eqs.(6)-(8), this terms relate to themselves and to each other as

$$\rho^{ij}_{ee} = \left(\rho^{ji}_{ee}\right)^\dagger \text{ and } \rho^{ij}_{eh} = -\rho^{ji}_{eh} \tag{16}$$
$$\rho^{ij}_{hh} = \delta_{ij} - \rho^{ji}_{ee} \text{ and } \rho^{ij}_{he} = \left(\rho^{ji}_{eh}\right)^\dagger \tag{17}$$

Moreover, accounting for the additional spin orbital quantum number, the Nambu-spinor corresponds instead to the 4-spinor

$$\check{\boldsymbol{c}}^\dagger_i = \begin{pmatrix} \boldsymbol{c}^\dagger_i & \boldsymbol{c}_i \end{pmatrix} = \begin{pmatrix} c^\dagger_{i\uparrow} & c^\dagger_{i\downarrow} & c_{i\uparrow} & c_{i\downarrow} \end{pmatrix} \tag{18}$$

such that each composite rDM is a matrix over orbital space, reading explicitly as

$$\check{\boldsymbol{\rho}}_{ij} = \langle \check{\boldsymbol{c}}^\dagger_j \otimes \check{\boldsymbol{c}}_i \rangle = \begin{pmatrix} \langle \boldsymbol{c}^\dagger_j \otimes \boldsymbol{c}_i \rangle & \langle \boldsymbol{c}_j \otimes \boldsymbol{c}_i \rangle \\ \langle \boldsymbol{c}^\dagger_j \otimes \boldsymbol{c}^\dagger_i \rangle & \langle \boldsymbol{c}_j \otimes \boldsymbol{c}^\dagger_i \rangle \end{pmatrix} \tag{19}$$
$$\equiv \begin{pmatrix} \boldsymbol{\rho}^{ij}_{ee} & \boldsymbol{\rho}^{ij}_{eh} \\ \boldsymbol{\rho}^{ij}_{he} & \boldsymbol{\rho}^{ij}_{hh} \end{pmatrix} \equiv \left(\begin{array}{cc|cc} \rho^{i\uparrow j\uparrow}_{ee} & \rho^{i\uparrow j\downarrow}_{ee} & \rho^{i\uparrow j\uparrow}_{eh} & \rho^{i\uparrow j\downarrow}_{eh} \\ \rho^{i\downarrow j\uparrow}_{ee} & \rho^{i\downarrow j\downarrow}_{ee} & \rho^{i\downarrow j\uparrow}_{eh} & \rho^{i\downarrow j\downarrow}_{eh} \\ \hline \rho^{i\uparrow j\uparrow}_{he} & \rho^{i\uparrow j\downarrow}_{he} & \rho^{i\uparrow j\uparrow}_{hh} & \rho^{i\uparrow j\downarrow}_{hh} \\ \rho^{i\downarrow j\uparrow}_{he} & \rho^{i\downarrow j\downarrow}_{he} & \rho^{i\downarrow j\uparrow}_{hh} & \rho^{i\downarrow j\downarrow}_{hh} \end{array}\right)$$

and relating to themselves and to each other as

$$\boldsymbol{\rho}^{ij}_{ee} = \left(\boldsymbol{\rho}^{ji}_{ee}\right)^\dagger \tag{20}$$
$$\boldsymbol{\rho}^{ij}_{eh} = -\left(\boldsymbol{\rho}^{ji}_{eh}\right)^T \tag{21}$$
$$\boldsymbol{\rho}^{ij}_{hh} = \boldsymbol{\delta}_{ij} - \left(\boldsymbol{\rho}^{ji}_{ee}\right)^T \tag{22}$$
$$\boldsymbol{\rho}^{ij}_{he} = \left(\boldsymbol{\rho}^{ji}_{eh}\right)^\dagger \tag{23}$$

To clarify possible misinterpretations of the notation, see that the the underlying electron-hole structure of an object is being concealed with the check notation while the underlying spin structure of an *object* is being concealed within the bold notation. The bold notation of a composite *index* $\boldsymbol{i} \equiv (i, s_i)$ does not underlies the objects spin structure, so beware the differences between $\rho^{\boldsymbol{ij}}_{ee} = \rho^{is_ijs_j}_{ee}$ and $\boldsymbol{\rho}^{ij}_{ee} = [\ \rho^{i\uparrow j\uparrow}_{ee}\ \ \rho^{i\uparrow j\downarrow}_{ee}\ ;\ \rho^{i\downarrow j\uparrow}_{ee}\ \ \rho^{i\downarrow j\downarrow}_{ee}\ ]$. The notation $\boldsymbol{\rho}^{\boldsymbol{ij}}_{ee}$ is not applicable for now since we are considering only spin and no other orbital degree of freedom. See that, for example, in a spinless case we would write $\check{\rho}^{ij} = [\ \rho^{ij}_{ee}\ \ \rho^{ij}_{eh}\ ;\ \rho^{ij}_{he}\ \ \rho^{ij}_{hh}\ ]$.

B. Nambu mean-field Hamiltonian

We start by solving for the purely electronic rDM equation of motions in the Heisenberg picture of quantum mechanics, where the fermionic operators evolve accordingly to the Heisenberg equation. We have

$$\frac{d}{dt} \rho^{\boldsymbol{ij}}_{ee} = \frac{\imath}{\hbar} \left\langle \left[H, c^\dagger_{\boldsymbol{j}} \right] c_{\boldsymbol{i}} \right\rangle + \frac{i}{\hbar} \left\langle c^\dagger_{\boldsymbol{j}} \left[H, c_{\boldsymbol{i}} \right] \right\rangle \tag{24}$$

with H the Hamiltonian in Eq.(11) and $\imath$ the imaginary unit. The time dependency in the fermionic operators is being omitted for compactness.

Making use of the fermionic anti-commutator properties, these commutators read, respectively,

$$[H, c^\dagger_{\boldsymbol{j}}] = \sum_{\boldsymbol{\alpha\beta}} H^{\boldsymbol{\alpha\beta}}_0 \left[c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\beta}}, c^\dagger_{\boldsymbol{j}} \right] + \frac{1}{2} \sum_{\boldsymbol{\alpha\beta}} v^{\alpha\beta} \left[c^\dagger_{\boldsymbol{\alpha}} c^\dagger_{\boldsymbol{\beta}} c_{\boldsymbol{\beta}} c_{\boldsymbol{\alpha}}, c^\dagger_{\boldsymbol{j}} \right]$$
$$[H, c_{\boldsymbol{i}}] = \sum_{\boldsymbol{\alpha\beta}} H^{\boldsymbol{\alpha\beta}}_0 \left[c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\beta}}, c_{\boldsymbol{i}} \right] + \frac{1}{2} \sum_{\boldsymbol{\alpha\beta}} v^{\alpha\beta} \left[c^\dagger_{\boldsymbol{\alpha}} c^\dagger_{\boldsymbol{\beta}} c_{\boldsymbol{\beta}} c_{\boldsymbol{\alpha}}, c_{\boldsymbol{i}} \right]$$

The commutators reading

$$\left[c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\beta}}, c^\dagger_j\right] = c^\dagger_{\boldsymbol{\alpha}} \delta_{\boldsymbol{\beta j}} \tag{25}$$
$$\left[c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\beta}}, c_{\boldsymbol{i}}\right] = -c_{\boldsymbol{\beta}} \delta_{\boldsymbol{i\alpha}} \tag{26}$$
$$\left[c^\dagger_{\boldsymbol{\alpha}} c^\dagger_{\boldsymbol{\beta}} c_{\boldsymbol{\beta}} c_{\boldsymbol{\alpha}}, c^\dagger_{\boldsymbol{j}}\right] = c^\dagger_{\boldsymbol{\alpha}} c^\dagger_{\boldsymbol{\beta}} c_{\boldsymbol{\beta}} \delta_{\boldsymbol{\alpha j}} - c^\dagger_{\boldsymbol{\alpha}} c^\dagger_{\boldsymbol{\beta}} c_{\boldsymbol{\alpha}} \delta_{\boldsymbol{\beta j}} \tag{27}$$
$$\left[c^\dagger_{\boldsymbol{\alpha}} c^\dagger_{\boldsymbol{\beta}} c_{\boldsymbol{\beta}} c_{\boldsymbol{\alpha}}, c_{\boldsymbol{i}}\right] = c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\beta}} c_{\boldsymbol{\alpha}} \delta_{\boldsymbol{\beta i}} - c^\dagger_{\boldsymbol{\beta}} c_{\boldsymbol{\beta}} c_{\boldsymbol{\alpha}} \delta_{\boldsymbol{i\alpha}} \tag{28}$$

where we used that

$$[AB, Z] = A\{B, Z\} - \{Z, A\} B \tag{29}$$
$$\begin{aligned}[ABCD, Z] =& AB\left(C\{D, Z\} - \{Z, C\} D\right) \\ &+ \left(A\{B, Z\} - \{Z, A\} B\right) CD\end{aligned} \tag{30}$$

The complete Heisenberg commutators then yield

$$\begin{aligned}[H, c^\dagger_{\boldsymbol{j}}] &= \sum_{\boldsymbol{\alpha}} H_0^{\boldsymbol{\alpha j}} c^\dagger_{\boldsymbol{\alpha}} + \frac{1}{2}\sum_{\boldsymbol{\beta}} v^{j\beta} c^\dagger_{\boldsymbol{j}} c^\dagger_{\boldsymbol{\beta}} c_{\boldsymbol{\beta}} - \frac{1}{2}\sum_{\boldsymbol{\alpha}} v^{\alpha j} c^\dagger_{\boldsymbol{\alpha}} c^\dagger_{\boldsymbol{j}} c_{\boldsymbol{\alpha}} \\ &= \sum_{\boldsymbol{\alpha}} H_0^{\boldsymbol{\alpha j}} c^\dagger_{\boldsymbol{\alpha}} + \frac{1}{2}\sum_{\boldsymbol{\alpha}} v^{\alpha j}\left(c^\dagger_{\boldsymbol{j}} c^\dagger_{\boldsymbol{\alpha}} - c^\dagger_{\boldsymbol{\alpha}} c^\dagger_{\boldsymbol{j}}\right) c_{\boldsymbol{\alpha}}\end{aligned} \tag{31}$$

$$\begin{aligned}[H, c_{\boldsymbol{i}}] &= -\sum_{\boldsymbol{\beta}} H_0^{\boldsymbol{i\beta}} c_{\boldsymbol{\beta}} + \frac{1}{2}\sum_{\boldsymbol{\alpha}} v^{\alpha i} c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{i}} c_{\boldsymbol{\alpha}} - \frac{1}{2}\sum_{\boldsymbol{\beta}} v^{i\beta} c^\dagger_{\boldsymbol{\beta}} c_{\boldsymbol{\beta}} c_{\boldsymbol{i}} \\ &= -\sum_{\boldsymbol{\alpha}} H_0^{\boldsymbol{i\alpha}} c_{\boldsymbol{\alpha}} + \frac{1}{2}\sum_{\boldsymbol{\alpha}} v^{\alpha i} c^\dagger_{\boldsymbol{\alpha}}\left(c_{\boldsymbol{i}} c_{\boldsymbol{\alpha}} - c_{\boldsymbol{\alpha}} c_{\boldsymbol{i}}\right)\end{aligned} \tag{32}$$

Substituting Eqs.(31) and (32) back into Eq.(**??**) yields

$$\begin{aligned}-\imath\hbar\frac{d}{dt}\rho_{ee}^{\boldsymbol{ij}} =& H_0^{\boldsymbol{\alpha j}}\left\langle c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{i}}\right\rangle - H_0^{\boldsymbol{i\alpha}}\left\langle c^\dagger_{\boldsymbol{j}} c_{\boldsymbol{\alpha}}\right\rangle \\ &+ \frac{1}{2} v^{\alpha j}\left(\left\langle c^\dagger_{\boldsymbol{j}} c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\alpha}} c_{\boldsymbol{i}}\right\rangle - \left\langle c^\dagger_{\boldsymbol{\alpha}} c^\dagger_{\boldsymbol{j}} c_{\boldsymbol{\alpha}} c_{\boldsymbol{i}}\right\rangle\right) \\ &+ \frac{1}{2} v^{\alpha i}\left(\left\langle c^\dagger_{\boldsymbol{j}} c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{i}} c_{\boldsymbol{\alpha}}\right\rangle - \left\langle c^\dagger_{\boldsymbol{j}} c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\alpha}} c_{\boldsymbol{i}}\right\rangle\right)\end{aligned}$$

Coming back to the rDM definitions and commutating the terms it reads

$$\begin{aligned}\imath\hbar\frac{d}{dt}\rho_{ee}^{\boldsymbol{ij}} =& -H_0^{\boldsymbol{\alpha j}}\rho_{ee}^{\boldsymbol{i\alpha}} + H_0^{\boldsymbol{i\alpha}}\rho_{ee}^{\boldsymbol{\alpha j}} \\ &- \left(v^{\alpha j} - v^{\alpha i}\right)\left\langle c^\dagger_{\boldsymbol{j}} c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\alpha}} c_{\boldsymbol{i}}\right\rangle\end{aligned} \tag{33}$$

Notice, however, that the interaction term will give rise to expectation values of four-operators. For this, we introduce a mean-field approximation where we assume the two-particle expectation value to simply behave as a product of two one-particle expectation values. From this mean-field decoupling we can then make use of *Wick's theorem*, yielding

$$\left\langle c^\dagger_{\boldsymbol{j}} c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\alpha}} c_{\boldsymbol{i}}\right\rangle \approx \rho_{he}^{\boldsymbol{\alpha j}}\rho_{eh}^{\boldsymbol{i\alpha}} - \rho_{ee}^{\boldsymbol{\alpha j}}\rho_{ee}^{\boldsymbol{i\alpha}} + \rho_{ee}^{\boldsymbol{ij}}\rho_{ee}^{\boldsymbol{\alpha\alpha}} \tag{34}$$

From this approximation, we defining the Hartree, Fock and Bogoliubov self-energies, themselves self-consistently dependent on the rDM, respectively as

$$\Sigma_H^{\boldsymbol{ij}} = \delta_{\boldsymbol{ij}}\sum_{\boldsymbol{\alpha}} v^{i\alpha}\rho_{ee}^{\boldsymbol{\alpha\alpha}} \tag{35}$$
$$\Sigma_F^{\boldsymbol{ij}} = -v^{ij}\rho_{ee}^{\boldsymbol{ij}} \tag{36}$$
$$\Sigma_B^{\boldsymbol{ij}} = v^{ij}\rho_{eh}^{\boldsymbol{ij}} \tag{37}$$

The interacting term of Eq.(**??**) yield

$$\begin{aligned}& v^{\alpha j}\left[\rho_{he}^{\boldsymbol{\alpha j}}\rho_{eh}^{\boldsymbol{i\alpha}} - \rho_{ee}^{\boldsymbol{\alpha j}}\rho_{ee}^{\boldsymbol{i\alpha}} + \rho_{ee}^{\boldsymbol{ij}}\rho_{ee}^{\boldsymbol{\alpha\alpha}}\right] \\ =& \left\{v^{\alpha j}\rho_{he}^{\boldsymbol{\alpha j}}\right\}\rho_{eh}^{\boldsymbol{i\alpha}} - \left\{v^{\alpha j}\rho_{ee}^{\boldsymbol{\alpha j}}\right\}\rho_{ee}^{\boldsymbol{i\alpha}} + \rho_{ee}^{\boldsymbol{ij}}\left\{v^{\alpha j}\rho_{ee}^{\boldsymbol{\alpha\alpha}}\right\} \\ =& \rho_{eh}^{\boldsymbol{i\alpha}}\left(-\Sigma_B^{\boldsymbol{\alpha j}}\right)^\dagger + \rho_{ee}^{\boldsymbol{i\alpha}}\Sigma_F^{\boldsymbol{\alpha j}} + \rho_{ee}^{\boldsymbol{ij}}\Sigma_H^{\boldsymbol{ii}} \\ =& \left\lceil -\boldsymbol{\rho}_{eh}^{ij}\left(-\boldsymbol{\Sigma}_B^{ji}\right)^\dagger + \boldsymbol{\rho}_{ee}^{ij}\boldsymbol{\Sigma}_F^{ij} + \boldsymbol{\rho}_{ee}^{ij}\boldsymbol{\Sigma}_H^{ij}\delta_{\boldsymbol{ij}}\right\rceil^{s_i s_j}\end{aligned} \tag{38}$$

$$\begin{aligned}& -v^{\alpha i}s\left[\rho_{he}^{\boldsymbol{\alpha j}}\rho_{eh}^{\boldsymbol{i\alpha}} - \rho_{ee}^{\boldsymbol{\alpha j}}\rho_{ee}^{\boldsymbol{i\alpha}} + \rho_{ee}^{\boldsymbol{ij}}\rho_{ee}^{\boldsymbol{\alpha\alpha}}\right] \\ =& -\left(\rho_{he}^{\boldsymbol{\alpha j}}\left\{v^{i\alpha}\rho_{eh}^{\boldsymbol{i\alpha}}\right\} + \rho_{ee}^{\boldsymbol{\alpha j}}\left\{-v^{i\alpha}\rho_{ee}^{\boldsymbol{i\alpha}}\right\} + \rho_{ee}^{\boldsymbol{ij}}\left\{v^{i\alpha}\rho_{ee}^{\boldsymbol{\alpha\alpha}}\right\}\right) \\ =& -\left(\Sigma_B^{\boldsymbol{i\alpha}}\rho_{he}^{\boldsymbol{\alpha j}} + \Sigma_F^{\boldsymbol{i\alpha}}\rho_{ee}^{\boldsymbol{\alpha j}} + \Sigma_H^{\boldsymbol{ii}}\rho_{ee}^{\boldsymbol{ij}}\right) \\ =& -\left\lceil \boldsymbol{\Sigma}_B^{ij}\boldsymbol{\rho}_{he}^{ij} + \boldsymbol{\Sigma}_F^{ij}\boldsymbol{\rho}_{ee}^{ij} + \boldsymbol{\rho}_{ee}^{ij}\boldsymbol{\Sigma}_H^{ij}\delta_{\boldsymbol{ij}}\right\rceil^{s_i s_j}\end{aligned} \tag{39}$$

where $\lceil\cdot\rceil^{s_i s_j}$ is the element at position $s_i s_j$, e.g $\lceil M\rceil^{\uparrow\uparrow} = M[1,1]$. Putting the three pieces together, and accounting for the complete spin structure, the purely electronic rDM EoM yields and shown in Eq.(42).

Note that, from the relations in Eqs.(16)-(17),

$$\Sigma_B^{\boldsymbol{ij}} = \left(v^{ij}\rho_{eh}^{\boldsymbol{ij}}\right) = v^{ij}\left(-\rho_{eh}^{\boldsymbol{ji}}\right) = -\Sigma_B^{\boldsymbol{ji}} \tag{40}$$
$$\left(\Sigma_B^{\boldsymbol{ji}}\right)^\dagger = \left(v^{ji}\rho_{eh}^{\boldsymbol{ji}}\right)^\dagger = \left(v^{ij}\rho_{he}^{\boldsymbol{ij}}\right) \overset{!}{=} -\left(\Sigma_B^{\boldsymbol{ij}}\right)^\dagger \tag{41}$$

The purely electronic rDM EoM then yields

$$\imath\hbar\frac{d}{dt}\boldsymbol{\rho}_{ee}^{ij} \approx \left[\boldsymbol{H}_{HF}^{ij}, \boldsymbol{\rho}_{ee}^{ij}\right] + \boldsymbol{\Sigma}_B^{ij}\cdot\boldsymbol{\rho}_{he}^{ij} - \boldsymbol{\rho}_{eh}^{ij}\cdot\left(\boldsymbol{\Sigma}_B^{ji}\right)^\dagger \tag{42}$$

where we have defined

$$\boldsymbol{H}_{HF}^{ij} = \boldsymbol{H}_0^{ij} + \boldsymbol{\Sigma}_H^{ij}\delta_{\boldsymbol{ij}} + \boldsymbol{\Sigma}_F^{ij} \tag{43}$$

Analogously for the anomalous rDM EoM, we obtain

$$\frac{d}{dt}\rho_{eh}^{\boldsymbol{ij}} = \frac{\imath}{\hbar}\left\langle [H, c_{\boldsymbol{j}}] c_{\boldsymbol{i}}\right\rangle + \frac{i}{\hbar}\left\langle c_{\boldsymbol{j}}[H, c_{\boldsymbol{i}}]\right\rangle \tag{44}$$
$$\left\langle [H, c_{\boldsymbol{j}}] c_{\boldsymbol{i}}\right\rangle = -\sum_{\boldsymbol{\alpha}} H_0^{\boldsymbol{j\alpha}}\rho_{eh}^{\boldsymbol{i\alpha}} - \sum_{\boldsymbol{\alpha}} v^{\alpha j}\left\langle c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\alpha}} c_{\boldsymbol{j}} c_{\boldsymbol{i}}\right\rangle \tag{45}$$
$$\left\langle c_{\boldsymbol{j}}[H, c_{\boldsymbol{i}}]\right\rangle = -\sum_{\boldsymbol{\alpha}} H_0^{\boldsymbol{i\alpha}}\rho_{eh}^{\boldsymbol{\alpha j}} - \sum_{\boldsymbol{\alpha}} v^{\alpha i}\left\langle c_{\boldsymbol{j}} c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\alpha}} c_{\boldsymbol{i}}\right\rangle \tag{46}$$
$$\left\langle c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\alpha}} c_{\boldsymbol{j}} c_{\boldsymbol{i}}\right\rangle \approx \rho_{ee}^{\boldsymbol{\alpha\alpha}}\rho_{eh}^{\boldsymbol{ij}} - \rho_{ee}^{\boldsymbol{j\alpha}}\rho_{eh}^{\boldsymbol{i\alpha}} + \rho_{ee}^{\boldsymbol{i\alpha}}\rho_{eh}^{\boldsymbol{j\alpha}} \tag{47}$$
$$\left\langle c_{\boldsymbol{j}} c^\dagger_{\boldsymbol{\alpha}} c_{\boldsymbol{\alpha}} c_{\boldsymbol{i}}\right\rangle \approx \rho_{hh}^{\boldsymbol{\alpha j}}\rho_{eh}^{\boldsymbol{i\alpha}} - \rho_{eh}^{\boldsymbol{\alpha j}}\rho_{ee}^{\boldsymbol{i\alpha}} + \rho_{eh}^{\boldsymbol{ij}}\rho_{ee}^{\boldsymbol{\alpha\alpha}} \tag{48}$$

and finally

$$i\hbar\frac{d}{dt}\boldsymbol{\rho}^{\boldsymbol{ij}}_{eh} \approx \boldsymbol{H}^{ij}_{HF}\cdot\boldsymbol{\rho}^{ij}_{eh} + \boldsymbol{\rho}^{ij}_{eh}\cdot\left(\boldsymbol{H}^{ij}_{HF}\right)^T + \boldsymbol{\Sigma}^{ij}_B\cdot\boldsymbol{\rho}^{ij}_{hh} - \boldsymbol{\rho}^{ij}_{ee}\cdot\boldsymbol{\Sigma}^{ij}_B \tag{49}$$

Finally, as introduced in Eqs.(88)-(**??**), we can represent the Nambu rDM EoM in terms of an effective Bogoliubov-de Gennes (BdG) Hamiltonian $\check{H}$ as simply as

$$\imath\hbar\frac{d}{dt}\check{\boldsymbol{\rho}}_{ij} = \left[\left(\check{\boldsymbol{H}}^{ij}_0 + \check{\boldsymbol{\Sigma}}^{ij}\right), \check{\boldsymbol{\rho}}_{ij}\right] \tag{50}$$

$$\check{\boldsymbol{H}}^{ij}_0 = \begin{pmatrix} \boldsymbol{H}^{ij}_0 & 0 \\ 0 & -\left(\boldsymbol{H}^{ji}_0\right)^T \end{pmatrix} \tag{51}$$

$$\check{\boldsymbol{\Sigma}}^{ij} = \begin{pmatrix} \boldsymbol{\Sigma}^{ij}_H + \boldsymbol{\Sigma}^{ij}_F & \boldsymbol{\Sigma}^{ij}_B \\ \left(\boldsymbol{\Sigma}^{ji}_B\right)^\dagger & -\left(\boldsymbol{\Sigma}^{ji}_H + \boldsymbol{\Sigma}^{ji}_F\right)^T \end{pmatrix} \tag{52}$$

It would be useful if we could express $\check{\boldsymbol{\Sigma}}$ more compactly in terms of $\check{\boldsymbol{\rho}}$. For this, and accounting for their spin structure, we re-express the Hartree term as

$$\begin{aligned}
\boldsymbol{\Sigma}^{ij}_H =& \boldsymbol{\delta}_{ij}\sum_{\boldsymbol{\alpha}} v^{i\alpha}\rho^{\boldsymbol{\alpha\alpha}}_{ee} \\
=& \delta_{ij}\sigma_0\sum_{\alpha} v^{i\alpha}\sum_{s_\alpha}\rho^{\alpha s_\alpha \alpha s_\alpha}_{ee} \\
=& \delta_{ij}\sigma_0\sum_{\alpha} v^{i\alpha}\left(\rho^{\alpha\uparrow\alpha\uparrow}_{ee} + \rho^{\alpha\downarrow\alpha\downarrow}_{ee}\right) \\
=& \delta_{ij}\sigma_0\sum_{\alpha} v^{i\alpha}\mathrm{Tr}\left(\boldsymbol{\rho}^{\alpha\alpha}_{ee}\right) && (53) \\
=& \delta_{ij}\sigma_0\sum_{\alpha} v^{i\alpha}\left[\frac{1}{2}\mathrm{Tr}\left([\tau_z\otimes\sigma_0]\check{\boldsymbol{\rho}}^{\alpha\alpha}\right) + 1\right] && (54) \\
\equiv& \frac{1}{2}\delta_{ij}\sigma_0\sum_{\alpha} v^{i\alpha}\mathrm{Tr}\left([\tau_z\otimes\sigma_0]\check{\boldsymbol{\varrho}}^{\alpha\alpha}\right) && (55)
\end{aligned}$$

with σ and τ as Pauli matrices but operating in their respectively spin and electron-hole subspaces the Hamiltonian and $\check{\boldsymbol{\varrho}}$ (var rho instead of rho) a newly defined BdG symmetric object:

$$\begin{aligned}
\check{\boldsymbol{\varrho}}^{ij} =& \begin{pmatrix} \boldsymbol{\rho}^{ij}_{ee} & \boldsymbol{\rho}^{ij}_{eh} \\ \left(\boldsymbol{\rho}^{ji}_{eh}\right)^\dagger & -\left(\boldsymbol{\rho}^{ji}_{ee}\right)^T \end{pmatrix} \\
=& \check{\boldsymbol{\rho}}^{ij} - \left[\frac{1}{2}\left(\tau_0 - \tau_z\right)\otimes\sigma_0\right] && (56)
\end{aligned}$$

Likewise, the Fock and Bogoliubov term, accounting for their spin structure, read as

$$\boldsymbol{\Sigma}^{ij}_F = -v^{ij}\boldsymbol{\rho}^{ij}_{ee} \tag{57}$$

$$\boldsymbol{\Sigma}^{ij}_B = v^{ij}\boldsymbol{\rho}^{ij}_{eh} \tag{58}$$

but can be re-expressed together in terms of the Nambu rDM as

$$\begin{aligned}
\boldsymbol{\Sigma}^{ij}_F + \boldsymbol{\Sigma}^{ij}_B &= -v^{ij}[\tau_z\otimes\sigma_0]\check{\boldsymbol{\rho}}_{ij}[\tau_z\otimes\sigma_0] \\
&= -v^{ij}[\tau_z\otimes\sigma_0]\check{\boldsymbol{\varrho}}_{ij}[\tau_z\otimes\sigma_0] && (59)
\end{aligned}$$

We can then compactly rewrite the Nambu mean field Hamiltonian as

$$\begin{aligned}
\check{\boldsymbol{\Sigma}}^{ij} =& \frac{1}{2}\delta_{ij}[\tau_z\otimes\sigma_0]\sum_{\alpha} v^{i\alpha}\mathrm{Tr}\left([\tau_z\otimes\sigma_0]\check{\boldsymbol{\varrho}}^{\alpha\alpha}\right) \\
&- v^{ij}[\tau_z\otimes\sigma_0]\check{\boldsymbol{\varrho}}^{ij}[\tau_z\otimes\sigma_0] && (60)
\end{aligned}$$

See that, apart from the Nambu/BdG symmetries of Eq.(52), there are additional constraint: the Hartree and Fock terms inherent the symmetry from Eq.(20), i.e $\boldsymbol{\Sigma}^{ji}_{H/F} = \left(\boldsymbol{\Sigma}^{ij}_{H/F}\right)^\dagger$ and the Bogoliubov term the symmetry from Eq.(21), i.e $\boldsymbol{\Sigma}^{ij}_B = -\left(\boldsymbol{\Sigma}^{ji}_B\right)^T$. From these constrains one can then see that

$$\begin{aligned}
&-[\tau_x\otimes\sigma_0]\left(\check{\boldsymbol{\Sigma}}^{ji}\right)^*[\tau_x\otimes\sigma_0] \\
&= \begin{pmatrix} -\left(\boldsymbol{\Sigma}^{ji}_{22}\right)^* & -\left(\boldsymbol{\Sigma}^{ji}_{21}\right)^* \\ -\left(\boldsymbol{\Sigma}^{ji}_{12}\right)^* & -\left(\boldsymbol{\Sigma}^{ji}_{11}\right)^* \end{pmatrix} = \check{\boldsymbol{\Sigma}}^{ij} && (61)
\end{aligned}$$

where $\left\{\check{\boldsymbol{\Sigma}}^{ij}\right\}^*$ terms reads explicitly as

$$\begin{aligned}
&\begin{pmatrix} \left\{\left[\boldsymbol{\Sigma}^{ji}_H\right]^\dagger + \left[\boldsymbol{\Sigma}^{ji}_F\right]^\dagger\right\}^* & \left\{-\left[\boldsymbol{\Sigma}^{ji}_B\right]^T\right\}^* \\ \left\{\left(-\left[\boldsymbol{\Sigma}^{ij}_B\right]^T\right)^\dagger\right\}^* & \left\{-\left(\left[\boldsymbol{\Sigma}^{ij}_H\right]^\dagger + \left[\boldsymbol{\Sigma}^{ij}_F\right]^\dagger\right)^T\right\}^* \end{pmatrix} \\
&= \begin{pmatrix} \left(\boldsymbol{\Sigma}^{ji}_H + \boldsymbol{\Sigma}^{ji}_F\right)^T & -\left(\boldsymbol{\Sigma}^{ji}_B\right)^\dagger \\ -\boldsymbol{\Sigma}^{ij}_B & -\left(\boldsymbol{\Sigma}^{ij}_H + \boldsymbol{\Sigma}^{ij}_F\right) \end{pmatrix} && (62)
\end{aligned}$$

All these symmetries relations can be summarized as

$$\check{\boldsymbol{\Sigma}}^{ij} = \left(\check{\boldsymbol{\Sigma}}^{ji}\right)^\dagger \tag{63}$$

$$\check{\boldsymbol{\Sigma}}^{ij} = -[\tau_x\otimes\sigma_0]\left(\check{\boldsymbol{\Sigma}}^{ji}\right)^*[\tau_x\otimes\sigma_0] \tag{64}$$

C. Orbital-dependent interactions

We now generalize the interaction model to include spin-spin interactions with orbital matrix elements $Q_{s_i s_i'}$ with $Q_{s_i s_i'} = Q_{s_i' s_i}$. The charge-charge interaction is recovered with $\check{\boldsymbol{Q}} = [\tau_z\otimes\sigma_0]$. In this context, see that the potential as it is written Eq.(3) is no longer true, but should read instead as

$$V_{\boldsymbol{j'i'}}^{\boldsymbol{ij}} \approx Q_{s_i s_i'} v^{ij} Q_{s_j s_j'} \delta_{ii'} \delta_{jj'} \tag{65}$$

As intended, the spurious interaction

$$\frac{1}{2} \sum_{is_i} \sum_{s_j'} \left(c_{is_i}^\dagger \left. \boldsymbol{Q}^2 \right|_{s_i s_j'} c_{is_j'} \right) v^{ii} \tag{66}$$

cancel out when writing the Hamiltonian it it's normal-ordered form leaving us only with

$$H_{\text{int}} = \frac{1}{2} \sum_{is_i} \sum_{js_j} \sum_{s_i' s_j'} c_{is_i}^\dagger c_{js_j}^\dagger \left\{ Q_{s_i s_i'} v^{ij} Q_{s_j s_j'} \right\} c_{js_j'} c_{is_i'}$$

From Eq.(53), (57), (58), the Hartree-Fock-Bogoliubov self-energies considering orbital-dependent interactions read respectively as

$$\boldsymbol{\Sigma}_H^{ij} = \delta_{ij} \boldsymbol{Q} \sum_\alpha v^{i\alpha} \text{Tr} \left(\boldsymbol{\rho}_{ee}^{\alpha\alpha} \right) \tag{67}$$

$$\boldsymbol{\Sigma}_F^{ij} = - v^{ij} \boldsymbol{Q} \boldsymbol{\rho}_{ee}^{ij} \boldsymbol{Q}^T \tag{68}$$

$$\boldsymbol{\Sigma}_B^{ij} = v^{ij} \boldsymbol{Q} \boldsymbol{\rho}_{eh}^{ij} \boldsymbol{Q}^T \tag{69}$$

and thus, the Nambu self-energy becomes

$$\check{\boldsymbol{\Sigma}}^{ij} = \frac{1}{2} \delta_{ij} \check{\boldsymbol{Q}} \sum_\alpha v^{i\alpha} \text{Tr} \left(\check{\boldsymbol{Q}} \check{\boldsymbol{\varrho}}^{\alpha\alpha} \right) - v^{ij} \check{\boldsymbol{Q}} \check{\boldsymbol{\varrho}}^{ij} \check{\boldsymbol{Q}} \tag{70}$$

1. Alternate Nambu basis

One may define the Nambu spinor differently. For example, instead of $\check{\boldsymbol{c}}_i^\dagger$ in Eq.(18), there is also common to encounter the so-called rotated basis where

$$\bar{\boldsymbol{c}}_i^\dagger = \left(\begin{array}{cc} \boldsymbol{c}_i^\dagger & [\imath \sigma_y \boldsymbol{c}_i] \end{array} \right) = \left(\begin{array}{cccc} c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger & c_{i\downarrow} & -c_{i\uparrow} \end{array} \right) \tag{71}$$

These relate to the previous choice of basis as

$$\bar{\boldsymbol{c}}_i = \bar{\boldsymbol{\mathcal{U}}} \check{\boldsymbol{c}}_i \Leftrightarrow \check{\boldsymbol{c}}_i = \bar{\boldsymbol{\mathcal{U}}}^\dagger \bar{\boldsymbol{c}}_i \tag{72}$$

$$\bar{\boldsymbol{c}}_i^\dagger = \check{\boldsymbol{c}}_i^\dagger \bar{\boldsymbol{\mathcal{U}}}^\dagger \Leftrightarrow \check{\boldsymbol{c}}_i^\dagger = \bar{\boldsymbol{c}}_i^\dagger \bar{\boldsymbol{\mathcal{U}}} \tag{73}$$

with $\bar{\boldsymbol{\mathcal{U}}}$ is a unitary matrix (i.e $\bar{\boldsymbol{\mathcal{U}}}^\dagger \bar{\boldsymbol{\mathcal{U}}} = \bar{\boldsymbol{\mathcal{U}}} \bar{\boldsymbol{\mathcal{U}}}^\dagger = \mathbb{1}$) reading

$$\bar{\boldsymbol{\mathcal{U}}} = \begin{pmatrix} \sigma_0 & 0 \\ 0 & \imath \sigma_y \end{pmatrix} = \left(\begin{array}{cc|cc} +1 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 \\ \hline 0 & 0 & 0 & +1 \\ 0 & 0 & -1 & 0 \end{array} \right) \tag{74}$$

The rotated basis Nambu rDMs, explicitly reading

$$\begin{aligned} \bar{\boldsymbol{\rho}}_{ij} &= \langle \bar{\boldsymbol{c}}_j^\dagger \otimes \bar{\boldsymbol{c}}_i \rangle \\ &= \begin{pmatrix} \langle \boldsymbol{c}_j^\dagger \otimes \boldsymbol{c}_i \rangle & \langle [\imath \sigma_y \boldsymbol{c}_j] \otimes \boldsymbol{c}_i \rangle \\ \langle \boldsymbol{c}_j^\dagger \otimes [\imath \sigma_y \boldsymbol{c}_i]^\dagger \rangle & \langle [\imath \sigma_y \boldsymbol{c}_j] \otimes [\imath \sigma_y \boldsymbol{c}_i]^\dagger \rangle \end{pmatrix} \\ &= \left(\begin{array}{cc|cc} \rho_{ee}^{i\uparrow j\uparrow} & \rho_{ee}^{i\uparrow j\downarrow} & \rho_{eh}^{i\uparrow j\downarrow} & -\rho_{eh}^{i\uparrow j\uparrow} \\ \rho_{ee}^{i\downarrow j\uparrow} & \rho_{ee}^{i\downarrow j\downarrow} & \rho_{eh}^{i\downarrow j\downarrow} & -\rho_{eh}^{i\downarrow j\uparrow} \\ \hline \rho_{he}^{i\downarrow j\uparrow} & \rho_{he}^{i\downarrow j\downarrow} & \rho_{hh}^{i\downarrow j\downarrow} & -\rho_{hh}^{i\downarrow j\uparrow} \\ -\rho_{he}^{i\uparrow j\uparrow} & -\rho_{he}^{i\uparrow j\downarrow} & -\rho_{hh}^{i\uparrow j\downarrow} & \rho_{hh}^{i\uparrow j\uparrow} \end{array} \right) \end{aligned}$$

can then be expressed also in terms of $\bar{\boldsymbol{\mathcal{U}}}$ as

$$\bar{\boldsymbol{\rho}}_{ij} = \langle \bar{\boldsymbol{c}}_j^\dagger \otimes \bar{\boldsymbol{c}}_i \rangle = \langle \check{\boldsymbol{c}}_i^\dagger \bar{\boldsymbol{\mathcal{U}}}^\dagger \otimes \bar{\boldsymbol{\mathcal{U}}} \check{\boldsymbol{c}}_i \rangle = \bar{\boldsymbol{\mathcal{U}}} \check{\boldsymbol{\rho}}_{ij} \bar{\boldsymbol{\mathcal{U}}}^\dagger \tag{75}$$

Likewise, the matrix for the Nambu $\boldsymbol{Q}$ becomes $\bar{\boldsymbol{Q}} = \bar{\boldsymbol{\mathcal{U}}} \check{\boldsymbol{Q}} \bar{\boldsymbol{\mathcal{U}}}^\dagger$. Since the last term of $\check{\boldsymbol{\varrho}}$ in Eq.(56) transforms into itself, then it also follows that $\bar{\boldsymbol{\varrho}} = \bar{\boldsymbol{\mathcal{U}}} \check{\boldsymbol{\varrho}} \bar{\boldsymbol{\mathcal{U}}}^\dagger$ and thus $\bar{\boldsymbol{\Sigma}}^{ij} = \bar{\boldsymbol{\mathcal{U}}} \check{\boldsymbol{\Sigma}}^{ij} \bar{\boldsymbol{\mathcal{U}}}^\dagger$ as in Eq.(60):

$$\bar{\boldsymbol{\Sigma}}^{ij} = \frac{1}{2} \delta_{ij} \bar{\boldsymbol{Q}} \sum_\alpha v^{i\alpha} \text{Tr} \left(\bar{\boldsymbol{Q}} \bar{\boldsymbol{\varrho}}^{\alpha\alpha} \right) - v^{ij} \bar{\boldsymbol{Q}} \bar{\boldsymbol{\varrho}}^{ij} \bar{\boldsymbol{Q}} \tag{76}$$

where we used that $\bar{\boldsymbol{\mathcal{U}}}$ is unitary and the cyclic property of the trace

$$\text{Tr} \left(\bar{\boldsymbol{\mathcal{U}}}^\dagger \bar{\boldsymbol{Q}} \bar{\boldsymbol{\varrho}}^{\alpha\alpha} \bar{\boldsymbol{\mathcal{U}}} \right) = \text{Tr} \left(\bar{\boldsymbol{\mathcal{U}}} \bar{\boldsymbol{\mathcal{U}}}^\dagger \bar{\boldsymbol{Q}} \bar{\boldsymbol{\varrho}}^{\alpha\alpha} \right) = \text{Tr} \left(\bar{\boldsymbol{Q}} \bar{\boldsymbol{\varrho}}^{\alpha\alpha} \right) \tag{77}$$

As a result of this transformation the Nambu symmetries expressed in Eq.(52) become

$$\bar{\boldsymbol{\Sigma}}^{ij} = \begin{pmatrix} \boldsymbol{\Sigma}_H^{ij} + \boldsymbol{\Sigma}_F^{ij} & -\imath \boldsymbol{\Sigma}_B^{ij} \sigma_y \\ \left(-\imath \boldsymbol{\Sigma}_B^{ji} \sigma_y \right)^\dagger & -\sigma_y \left(\boldsymbol{\Sigma}_H^{ji} + \boldsymbol{\Sigma}_F^{ji} \right)^T \sigma_y \end{pmatrix} \tag{78}$$

Using the fact that $\bar{\boldsymbol{\mathcal{U}}}$ is unitary, Eq.(64) then becomes

$$\begin{aligned} \bar{\boldsymbol{\Sigma}}^{ij} &= \bar{\boldsymbol{\mathcal{U}}} \check{\boldsymbol{\Sigma}}^{ij} \bar{\boldsymbol{\mathcal{U}}}^\dagger \\ &= - \left[\bar{\boldsymbol{\mathcal{U}}} [\tau_x \otimes \sigma_0] \bar{\boldsymbol{\mathcal{U}}}^\dagger \right] \left[\bar{\boldsymbol{\mathcal{U}}} \left(\check{\boldsymbol{\Sigma}}^{ij} \right)^* \bar{\boldsymbol{\mathcal{U}}}^\dagger \right] \left[\bar{\boldsymbol{\mathcal{U}}} [\tau_x \otimes \sigma_0] \bar{\boldsymbol{\mathcal{U}}}^\dagger \right] \\ &= - [\tau_y \otimes \sigma_y] \left(\bar{\boldsymbol{\Sigma}}^{ij} \right)^* [\tau_y \otimes \sigma_y] \end{aligned}$$

where

$$\begin{aligned} &\bar{\boldsymbol{\mathcal{U}}} [\tau_x \otimes \sigma_0] \bar{\boldsymbol{\mathcal{U}}}^\dagger \\ &= \begin{pmatrix} \sigma_0 & 0 \\ 0 & \imath \sigma_y \end{pmatrix} \begin{pmatrix} 0 & \sigma_0 \\ \sigma_0 & 0 \end{pmatrix} \begin{pmatrix} \sigma_0 & 0 \\ 0 & -\imath \sigma_y \end{pmatrix} \\ &= \begin{pmatrix} 0 & -\imath \sigma_y \\ \imath \sigma_y & 0 \end{pmatrix} = (-\imath \tau_y) \otimes (\imath \sigma_y) \end{aligned} \tag{79}$$

The Nambu symmetries relations for the rotated basis read as

$$\bar{\boldsymbol{\Sigma}}^{ij} = \left(\bar{\boldsymbol{\Sigma}}^{ji} \right)^\dagger \tag{80}$$

$$\bar{\boldsymbol{\Sigma}}^{ij} = - [\tau_y \otimes \sigma_y] \left(\bar{\boldsymbol{\Sigma}}^{ij} \right)^* [\tau_y \otimes \sigma_y] \tag{81}$$

D. Hubbard model

Consider, instead of the spinless potential from Eq.(4), a spinful Hubbard potential

$$v^{ij} = U\delta_{ij} \tag{82}$$

In this model, the original non-normal-ordered interaction Hamiltonian from Eq.(5) is instead

$$\begin{aligned}
H_{\text{int}} =& \frac{1}{2}\sum_{\boldsymbol{ij}} c^{\dagger}_{\boldsymbol{i}} c_{\boldsymbol{i}} v^{ij} c^{\dagger}_{\boldsymbol{j}} c_{\boldsymbol{j}} - \frac{1}{2}\sum_{\boldsymbol{i}} c^{\dagger}_{\boldsymbol{i}} c_{\boldsymbol{i}} v^{ii} \\
=& \frac{1}{2}\sum_{is_i}\sum_{is_j} c^{\dagger}_{is_i} c_{is_i} \{U\delta_{ij}\} c^{\dagger}_{js_j} c_{js_j} - \frac{1}{2}\sum_{is_i} c^{\dagger}_{is_i} c_{is_i} \{U\delta_{ii}\} \\
=& \frac{1}{2}U\sum_{is_i}\left[\left(c^{\dagger}_{is_i} c_{is_i} n_{i\uparrow} + c^{\dagger}_{is_i} c_{is_i} n_{i\downarrow}\right) - \left(n_{i\uparrow} + n_{i\downarrow}\right)\delta_{ii}\right] \\
=& \frac{1}{2}U\sum_{i}\left(n_{i\uparrow}n_{i\downarrow} + n_{i\downarrow}n_{i\uparrow}\right)
\end{aligned} \tag{83}$$

where $n_{is_i} = c^{\dagger}_{is_i} c_{is_i}$ is the number operator and

$$\left(n_{i\uparrow}n_{i\uparrow} - n_{i\uparrow}\delta_{ii}\right) + \left(n_{i\downarrow}n_{i\downarrow} - n_{i\downarrow}\delta_{ii}\right) = 0 \tag{84}$$

because $n_{is_i}n_{is_i} = (n_{is_i})^2 = n_{is_i}$ (there is or there is not an electron at site i and spin s_i, i.e $n_{is_i} = 0$ or 1). Using that

$$\begin{aligned}
n_{is_i}n_{i\bar{s}_i} &= c^{\dagger}_{is_i}\left\{c_{is_i}c^{\dagger}_{i\bar{s}_i}\right\}c_{i\bar{s}_i} = c^{\dagger}_{is_i}\left(\delta_{ii}\cancelto{0}{\delta_{s_i\bar{s}_i}} - c^{\dagger}_{i\bar{s}_i}c_{is_i}\right)c_{i\bar{s}_i} \\
&= -\left\{c^{\dagger}_{is_i}c^{\dagger}_{i\bar{s}_i}\right\}\left\{c_{is_i}c_{i\bar{s}_i}\right\} = -c^{\dagger}_{i\bar{s}_i}\left\{c^{\dagger}_{is_i}c_{i\bar{s}_i}\right\}c_{is_i} \\
&= n_{i\bar{s}_i}n_{is_i},
\end{aligned} \tag{85}$$

one can simply write

$$H_{\text{int}} \to H_U = U\sum_i n_{i\uparrow}n_{i\downarrow} \tag{86}$$

Also, see that by definition of the model, spurious interaction do not take part so there is no need to subtracting them preemptively. The Nambu self-energy term then reads

$$\begin{aligned}
\check{\boldsymbol{\Sigma}}^{ij}_U =& U\delta_{ij}\left(\frac{1}{2}[\tau_z\otimes\sigma_0]\mathrm{Tr}\left([\tau_z\otimes\sigma_0]\check{\boldsymbol{\varrho}}^{ii}\right)\right. \\
&\left. - [\tau_z\otimes\sigma_0]\check{\boldsymbol{\varrho}}^{ij}[\tau_z\otimes\sigma_0]\right)
\end{aligned} \tag{87}$$

Part II

Oreg-Lutchyn model

The Oreg-Lutchyn Majorana minimal model consists of a finite 1D semiconductor (SM) nanowire with strong spin-orbit coupling (SOC) α and a tunable chemical potential μ, in proximity of a superconductor (SC) of homogeneous pairing Δ, having a magnetic field B_z applied along it's length, defined as the $\hat{z}$ direction. The Rashba effect describes the coupling of an electric field E_x that breaks inversion symmetry breaking in the direction perpendicular to the wire, to the electron's spin, i.e $\propto (\imath\vec{\nabla}\times\hat{x})\cdot\vec{\sigma} = \imath\sigma_y\partial_z$ with $\vec{\sigma} = (\sigma_x,\, \sigma_y,\, \sigma_z)$. The Zeeman effect described the spin splitting due to the in-plane magnetic field B_z. The pairing term describes the Cooper pairs from BCS theory than could tunnel from the SM to the SC. The Hamiltonian describing this system can then be decomposed as

$$H = H_{\text{K}} + H_{\text{SOC}} + H_{\text{Z}} + H_{\text{SC}} \tag{88}$$

$$H_{\text{K}} = \sum_s c^{\dagger}_s\left(-\eta\partial_z^2 - \mu\right)c_s \tag{89}$$

$$H_{\text{SOC}} = \boldsymbol{c}^{\dagger}\left(\imath\alpha\sigma_y\partial_z\right)\boldsymbol{c} \tag{90}$$

$$H_{\text{Z}} = \boldsymbol{c}^{\dagger}\left(V_Z\sigma_z\right)\boldsymbol{c} \tag{91}$$

$$H_{\text{SC}} = \Delta\left(c^{\dagger}_{\downarrow}c^{\dagger}_{\uparrow} + \text{h.c.}\right) \tag{92}$$

with $c \equiv c(z)$, $c^{\dagger} \equiv c^{\dagger}(z)$ fermionic operators, $\eta = \hbar^2/2m^*$ with m^* the effective mass of the electrons and $V_{\text{Z}} = g_J\mu_{\text{B}}B_z/2$ the Zeeman potential with g_J the Landé gyromagnetic moment and μ_{B} Bohr's magneton. See that the representation of the SOC and Zeeman Hamiltonians in Eq.(90) and Eq.(91) respectively, make use of the fermion spinors introduced in the previous part. In the unrotated basis these read as

$$\boldsymbol{c}^{\dagger} = \begin{pmatrix} c^{\dagger}_{\uparrow} & c^{\dagger}_{\downarrow} \end{pmatrix} \text{ and } \boldsymbol{c} = \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow} \end{pmatrix}. \tag{93}$$

See that, if one wanted, we could also write the kinetic term in this fashion instead as $H_{\text{K}} = \boldsymbol{c}^{\dagger}(-\eta\partial_z^2 - \mu)\sigma_0\boldsymbol{c}$.

Let us consider a tight-binding such that where z is discretized and specified by a given lattice site i distancing from each other by the lattice constant $\delta_z \equiv a_0$. The discretized partial derivatives (in central differencing) follows as

$$\begin{aligned}
\partial_z c(z) &\to \frac{1}{2a_0}\left(c_{(i+1)} - c_{(i-1)}\right) \\
&= \frac{1}{2a_0}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}\begin{pmatrix} c_{(i-1)} \\ c_i \\ c_{(i+1)} \end{pmatrix}
\end{aligned} \tag{94}$$

and consequently

$$\begin{aligned}
\partial_z^2 c(z) &\to \frac{1}{a_0^2}\left(c_{(i+1)} - 2c_i + c_{(i-1)}\right). \\
&= \frac{1}{a_0^2}\begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix}\begin{pmatrix} c_{(i-1)} \\ c_i \\ c_{(i+1)} \end{pmatrix}
\end{aligned} \tag{95}$$

In this discretized space, one can check that

$$
\begin{aligned}
&c^\dagger(z)\left(-\eta\partial_z^2-\mu\right)c(z)\\
&\to\begin{pmatrix} c_{i-1}^\dagger & c_i^\dagger & c_{i+1}^\dagger\end{pmatrix}\begin{pmatrix}2t-\mu & -t & 0\\ -t & 2t-\mu & -t\\ 0 & -t & 2t-\mu\end{pmatrix}\begin{pmatrix}c_{i-1}\\ c_i\\ c_{i+1}\end{pmatrix}\\
&=\left(c_{i-1}^\dagger(2t-\mu)c_{i-1}-c_{i-1}^\dagger t c_i\right)\\
&\quad+\left(-c_i^\dagger t c_{i-1}+c_i^\dagger(2t-\mu)c_i-c_i^\dagger t c_{i+1}\right)\\
&\quad+\left(-c_{i+1}^\dagger t c_i+c_{i+1}^\dagger(2t-\mu)c_{i+1}\right)
\end{aligned}
\tag{96}
$$

and thus the kinetics term from Eq.(89) reads simply as

$$
H_\mathrm{K}=(2t-\mu)\sum_{is}c_{is}^\dagger c_{is}-t\sum_{\langle i,j\rangle s}c_{is}^\dagger c_{js}
\tag{97}
$$

with $t=\eta/a_0^2$ the hopping constant into $\langle i,j\rangle$ nearest-neighbouring sites. This terms corresponds to the onsite energies of the nearest-neighbouring sites and the back-and-forward hoppings between them, for both spins. Analogously, see that

$$
\begin{aligned}
&\boldsymbol{c}^\dagger(z)\imath\sigma_y\partial_z\boldsymbol{c}(z)\\
&\to\begin{pmatrix}\boldsymbol{c}_{i-1}^\dagger & \boldsymbol{c}_i^\dagger & \boldsymbol{c}_{i+1}^\dagger\end{pmatrix}\imath\sigma_y\begin{pmatrix}0 & 1 & 0\\ -1 & 0 & 1\\ 0 & -1 & 0\end{pmatrix}\begin{pmatrix}\boldsymbol{c}_{i-1}\\ \boldsymbol{c}_i\\ \boldsymbol{c}_{i+1}\end{pmatrix}\\
&=\boldsymbol{c}_{i-1}^\dagger\imath\sigma_y\boldsymbol{c}_i-\boldsymbol{c}_i^\dagger\imath\sigma_y\boldsymbol{c}_{i-1}+\boldsymbol{c}_i^\dagger\imath\sigma_y\boldsymbol{c}_{i+1}-\boldsymbol{c}_{i+1}^\dagger\imath\sigma_y\boldsymbol{c}_i\\
&=\left(c_{(i-1)\uparrow}^\dagger c_{i\downarrow}-c_{(i-1)\downarrow}^\dagger c_{i\uparrow}\right)-\left(c_{i\uparrow}^\dagger c_{(i-1)\downarrow}-c_{i\downarrow}^\dagger c_{(i-1)\uparrow}\right)\\
&\quad+\left(c_{i\uparrow}^\dagger c_{(i+1)\downarrow}-c_{i\downarrow}^\dagger c_{(i+1)\uparrow}\right)-\left(c_{(i+1)\uparrow}^\dagger c_{i\downarrow}-c_{(i+1)\downarrow}^\dagger c_{i\uparrow}\right)\\
&=\left(c_{(i-1)\uparrow}^\dagger c_{i\downarrow}+\mathrm{h.c.}\right)-\left(c_{(i-1)\downarrow}^\dagger c_{i\uparrow}+\mathrm{h.c.}\right)\\
&\quad+\left(c_{i\uparrow}^\dagger c_{(i+1)\downarrow}+\mathrm{h.c.}\right)-\left(c_{i\downarrow}^\dagger c_{(i+1)\uparrow}+\mathrm{h.c.}\right)
\end{aligned}
\tag{98}
$$

Thus the SOC term in Eq.(90) can be expressed as

$$
H_\mathrm{SOC}=\frac{\alpha}{2a_0}\sum_{\langle i,j\rangle}\left(c_{i\uparrow}^\dagger c_{j\downarrow}-c_{i\downarrow}^\dagger c_{j\uparrow}\right)+\mathrm{h.c.}
\tag{99}
$$

with $\bar{s}$ is the opposite spin of s. This terms corresponds to the back-and-forward interaction between opposites spins on nearest-neighbouring sites. Eq.(99) should be like I have, no? You have it slightly different.

On a related yet distinct note, see that one cannot express with just the spin-spinors $\boldsymbol{c}_i/\boldsymbol{c}_i^\dagger$ the pairing Hamiltonian in Eq.(92), as we did for all the other. For this we need to double the degrees of freedom through the Nambu-spinor, as introduced in the previous part. In the unrotated basis it reads

$$
\check{\boldsymbol{c}}_i^\dagger=\begin{pmatrix}\boldsymbol{c}_i^\dagger & \boldsymbol{c}_i\end{pmatrix}=\begin{pmatrix}c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger & c_{i\uparrow} & c_{i\downarrow}\end{pmatrix}
\tag{100}
$$

Within this (discretized) Nambu⊗spin space the pairing Hamiltonian can be rewritten as

$$
\check{\boldsymbol{H}}_\mathrm{SC}=\frac{1}{2}\Delta\sum_i\check{\boldsymbol{c}}_i^\dagger[\tau_y\otimes\sigma_y]\check{\boldsymbol{c}}_i
\tag{101}
$$

since, and making things explicit,

$$
\begin{aligned}
&\frac{1}{2}\check{\boldsymbol{c}}^\dagger[\tau_y\otimes\sigma_y]\check{\boldsymbol{c}}\\
=&\frac{1}{2}\begin{pmatrix}c_\uparrow^\dagger & c_\downarrow^\dagger & c_\uparrow & c_\downarrow\end{pmatrix}\left(\begin{array}{cc|cc}0 & 0 & 0 & -1\\ 0 & 0 & +1 & 0\\ \hline 0 & +1 & 0 & 0\\ -1 & 0 & 0 & 0\end{array}\right)\begin{pmatrix}c_\uparrow\\ c_\downarrow\\ c_\uparrow^\dagger\\ c_\downarrow^\dagger\end{pmatrix}\\
=&\frac{1}{2}\left(-c_\uparrow^\dagger c_\downarrow^\dagger+c_\downarrow^\dagger c_\uparrow^\dagger+c_\uparrow c_\downarrow-c_\downarrow c_\uparrow\right)\\
=&c_\downarrow^\dagger c_\uparrow^\dagger+\mathrm{h.c.}
\end{aligned}
\tag{102}
$$

Still do not fully understand why the code can just ignore the 1/2 factor. Rewrite the other Hamiltonians in the this Nambu⊗spin space is a simpler task because there is no mixing of eh components. Hence, the holeonic terms must just then the negative of the electronic terms, meaning that one just needs to expand the space according to $\tau_z\otimes$ the respective spin matrix.

As a resume, in the discretized Nambu⊗spin space the complete Hamiltonian reads as

$$
H=H_\mathrm{K}+H_\mathrm{SOC}+H_\mathrm{Z}+H_\mathrm{SC}
\tag{103}
$$

$$
H_\mathrm{K}=(2t-\mu)\sum_i\check{\boldsymbol{c}}_i^\dagger[\tau_z\otimes\sigma_0]\check{\boldsymbol{c}}_i-\frac{1}{2}t\sum_{\langle i,j\rangle}\check{\boldsymbol{c}}_i^\dagger[\tau_z\otimes\sigma_0]\check{\boldsymbol{c}}_j
\tag{104}
$$

$$
H_\mathrm{SOC}=\frac{\alpha}{2a_0}\sum_i\check{\boldsymbol{c}}_i^\dagger[\tau_z\otimes\imath\sigma_y]\check{\boldsymbol{c}}_j
\tag{105}
$$

$$
H_\mathrm{Z}=V_Z\sum_i\check{\boldsymbol{c}}_i^\dagger[\tau_z\otimes\sigma_z]\check{\boldsymbol{c}}_j
\tag{106}
$$

$$
H_\mathrm{SC}=\frac{1}{2}\Delta\sum_i\check{\boldsymbol{c}}_i^\dagger[\tau_y\otimes\sigma_y]\check{\boldsymbol{c}}_i
\tag{107}
$$

For a more comprehensive understanding, we show explicitly why this is the case, for example, for the kinetic term:

$$
\begin{aligned}
&\frac{1}{2}\check{\boldsymbol{c}}_i^\dagger[\tau_z\otimes\sigma_0]\check{\boldsymbol{c}}_j\\
=&\frac{1}{2}\begin{pmatrix}c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger & c_{i\uparrow} & c_{i\downarrow}\end{pmatrix}\left(\begin{array}{cc|cc}+1 & 0 & 0 & 0\\ 0 & +1 & 0 & 0\\ \hline 0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\end{array}\right)\begin{pmatrix}c_{j\uparrow}\\ c_{j\downarrow}\\ c_{j\uparrow}^\dagger\\ c_{j\downarrow}^\dagger\end{pmatrix}\\
=&\frac{1}{2}\left(c_{i\uparrow}^\dagger c_{j\uparrow}+c_{i\downarrow}^\dagger c_{j\downarrow}-c_{i\uparrow}c_{j\uparrow}^\dagger-c_{i\downarrow}c_{j\downarrow}^\dagger\right)\\
=&\begin{cases}\frac{1}{2}\left(c_{i\uparrow}^\dagger c_{j\uparrow}+c_{j\uparrow}^\dagger c_{i\uparrow}\right)+\frac{1}{2}\left(c_{i\downarrow}^\dagger c_{j\downarrow}+c_{j\downarrow}^\dagger c_{i\downarrow}\right) & \text{for } i\neq j\\ \left(c_{i\uparrow}^\dagger c_{i\uparrow}+c_{i\downarrow}^\dagger c_{i\downarrow}\right)-1 & \text{for } i=j\end{cases}\\
=&\begin{cases}\frac{1}{2}\sum_s c_{is}^\dagger c_{js}+\mathrm{h.c.} & \text{for } i\neq j\\ \sum_s c_{is}^\dagger c_{is}-1 & \text{for } i=j\end{cases}
\end{aligned}
\tag{108}
$$

noting that

$$
\frac{1}{2}\sum_s c_{is}^\dagger c_{js}+\mathrm{h.c.}=\sum_{\langle i,j\rangle s}c_{is}^\dagger c_{js}
$$

What about the $\delta_{ii}\delta_{\uparrow\uparrow}=\delta_{ii}\delta_{\downarrow\downarrow}=-1$ on the $i=j$ term?

ALTERNATIVE NAMBU BASIS

It is common for people to define instead the Nambu spinor in a rotated basis as such

$$\bar{\boldsymbol{c}}_i^\dagger = \begin{pmatrix} \boldsymbol{c}_i^\dagger & [i\sigma_y \boldsymbol{c}_i] \end{pmatrix} = \left(\begin{array}{cc|cc} c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger & c_{i\downarrow} & -c_{i\uparrow} \end{array} \right) \quad (109)$$

As also explained in section II.C.1 of the previous part, these basis' operators relate to each other as

$$\bar{\boldsymbol{c}}_i = \bar{\boldsymbol{\mathcal{U}}} \check{\boldsymbol{c}}_i \Leftrightarrow \check{\boldsymbol{c}}_i = \bar{\boldsymbol{\mathcal{U}}}^\dagger \bar{\boldsymbol{c}}_i \quad (110)$$

$$\bar{\boldsymbol{c}}_i^\dagger = \check{\boldsymbol{c}}_i^\dagger \bar{\boldsymbol{\mathcal{U}}}^\dagger \Leftrightarrow \check{\boldsymbol{c}}_i^\dagger = \bar{\boldsymbol{c}}_i^\dagger \bar{\boldsymbol{\mathcal{U}}} \quad (111)$$

and, consequently, for a generic $\check{\boldsymbol{M}}$ matrix,

$$\bar{\boldsymbol{M}} = \bar{\boldsymbol{\mathcal{U}}} \check{\boldsymbol{M}} \bar{\boldsymbol{\mathcal{U}}}^\dagger \quad (112)$$

with $\bar{\boldsymbol{\mathcal{U}}}$ is a unitary matrix (i.e $\bar{\boldsymbol{\mathcal{U}}}^\dagger \bar{\boldsymbol{\mathcal{U}}} = \bar{\boldsymbol{\mathcal{U}}} \bar{\boldsymbol{\mathcal{U}}}^\dagger = \mathbb{1}$)

$$\bar{\boldsymbol{\mathcal{U}}} = \begin{pmatrix} \sigma_0 & 0 \\ 0 & \imath\sigma_y \end{pmatrix} \quad (113)$$

Making use of Pauli matrices' property

$$\sigma_\alpha \sigma_\beta = \sigma = \sigma_0 \delta_{\alpha\beta} + i\varepsilon_{\alpha\beta\gamma}\sigma_\gamma \quad (114)$$

one can check that

$$H_{\mathrm{K}} : \bar{\boldsymbol{\mathcal{U}}} [\tau_z \otimes \sigma_0] \bar{\boldsymbol{\mathcal{U}}}^\dagger = [\tau_z \otimes \sigma_0] \quad (115)$$

$$H_{\mathrm{SOC}} : \bar{\boldsymbol{\mathcal{U}}} [\tau_z \otimes \imath\sigma_y] \bar{\boldsymbol{\mathcal{U}}}^\dagger = [\tau_z \otimes \imath\sigma_y] \quad (116)$$

$$H_{\mathrm{Z}} : \bar{\boldsymbol{\mathcal{U}}} [\tau_z \otimes \sigma_z] \bar{\boldsymbol{\mathcal{U}}}^\dagger = [\tau_z \otimes \sigma_z] \quad (117)$$

$$H_{\mathrm{SC}} : \bar{\boldsymbol{\mathcal{U}}} [\tau_y \otimes \sigma_y] \bar{\boldsymbol{\mathcal{U}}}^\dagger = [\tau_x \otimes \sigma_0] \quad (118)$$

meaning that, in this the rotated basis, only the pairing Hamiltonian has it's Pauli matrices changed. Concretely,

$$H_{\mathrm{SC}} = \frac{1}{2}\Delta \sum_i \bar{\boldsymbol{c}}_i^\dagger [\tau_x \otimes \sigma_0] \bar{\boldsymbol{c}}_i \quad (119)$$