

Supplementary notes on:

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

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Part I

Hartree-Fock-Bogoliubov mean-field theory

I. HAMILTONIAN DESCRIPTION

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

$$H = H_0 + H_{\text{int}} = \sum_{ij} c_i^\dagger H_0^{ij} c_j + \frac{1}{2} \sum_{ij} \sum_{i'j'} c_i^\dagger c_{i'} V_{j'i'}^{ij} c_j^\dagger c_{j'} \quad (1)$$

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

$$\mathbf{i} \equiv (i, s_i) \quad (2)$$

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 $\sum_{\mathbf{i}} = \sum_{s_i} \sum_i$ and $\delta_{ij} = \delta_{ij} \delta_{s_i s_j}$.

A. Wannier spinless potential

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

$$V_{j'i'}^{ij} \approx v^{ij} \delta_{ii'} \delta_{jj'} \quad (3)$$

mediated by a spinless electrostatic scalar potential

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

It follows that

$$H_{\text{int}} = \frac{1}{2} \sum_{ij} \sum_{i'j'} c_i^\dagger c_{i'} (v^{ij} \delta_{ii'} \delta_{jj'}) c_j^\dagger c_{j'} = \frac{1}{2} \sum_{ij} c_i^\dagger c_i v^{ij} c_j^\dagger c_j \quad (5)$$

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,

$$\{c_i, c_j^\dagger\} = c_i c_j^\dagger + c_j^\dagger c_i \quad (6)$$

$$\{c_i, c_j^\dagger\} = \{c_j^\dagger, c_i\} = \delta_{ij} \quad (7)$$

$$\{c_i, c_j\} = \{c_j^\dagger, c_i^\dagger\} = 0, \quad (8)$$

one obtains

$$H_{\text{int}} = \frac{1}{2} \sum_{ij} c_i^\dagger c_i v^{ij} c_j^\dagger c_j = \frac{1}{2} \sum_{ij} c_i^\dagger (\delta_{ij} - c_j^\dagger c_i) c_j v^{ij} = \frac{1}{2} c_i^\dagger c_i v^{ii} - \frac{1}{2} \sum_{ij} c_i^\dagger c_j^\dagger v^{ij} c_i c_j \quad (9)$$

See that from the normal ordering of H_{int} a non-physical spurious self-interaction term $1/2 c_i^\dagger c_i v^{ii}$ 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,

$$H_{\text{int}} - = \frac{1}{2} \sum_{\mathbf{i}} c_i^\dagger c_i v^{ii} \quad (10)$$

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

$$H = \sum_{ij} c_i^\dagger H_0^{ij} c_j + \frac{1}{2} \sum_{ij} c_i^\dagger c_j^\dagger v^{ij} c_j c_i \quad (11)$$

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:

$$H \approx H_0 + H_{\text{int}}^H + H_{\text{int}}^F + H_{\text{int}}^B \quad (12)$$

$$= \sum_{ij} \left[c_i^\dagger \left(H_0^{ij} + \Sigma_H^{ij} + \Sigma_F^{ij} \right) c_j + \frac{1}{2} \left(c_i^\dagger \Sigma_B^{ij} c_j^\dagger + h.c \right) \right].$$

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

$$\check{H} = \frac{1}{2} \sum_{ij} \check{c}_i \left(\check{H}_0^{ij} + \check{\Sigma}^{ij} \right) \check{c}_j, \quad (13)$$

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 $\rho_{ee} = \langle c_j^\dagger c_i \rangle$ 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,

$$\check{c}_i^\dagger = (c_i^\dagger \ c_i) \text{ and } \check{c}_i = \begin{pmatrix} c_i \\ c_i^\dagger \end{pmatrix} \quad (14)$$

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

$$\check{\rho}_{ij} = \langle \check{c}_j^\dagger \otimes \check{c}_i \rangle \quad (15)$$

$$= \begin{pmatrix} \langle c_j^\dagger c_i \rangle & \langle c_j c_i \rangle \\ \langle c_j^\dagger c_i^\dagger \rangle & \langle c_j c_i^\dagger \rangle \end{pmatrix} \equiv \begin{pmatrix} \rho_{ee}^{ij} & \rho_{eh}^{ij} \\ \rho_{he}^{ij} & \rho_{hh}^{ij} \end{pmatrix}$$

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

$$\rho_{ee}^{ij} = (\rho_{ee}^{ji})^\dagger \text{ and } \rho_{eh}^{ij} = -\rho_{eh}^{ji} \quad (16)$$

$$\rho_{hh}^{ij} = \delta_{ij} - \rho_{ee}^{ji} \text{ and } \rho_{he}^{ij} = (\rho_{eh}^{ji})^\dagger \quad (17)$$

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

$$\check{c}_i^\dagger = (c_i^\dagger \ c_i) = \begin{pmatrix} c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger & c_{i\uparrow} & c_{i\downarrow} \end{pmatrix} \quad (18)$$

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

$$\check{\rho}_{ij} = \langle \check{c}_j^\dagger \otimes \check{c}_i \rangle = \begin{pmatrix} \langle c_j^\dagger \otimes c_i \rangle & \langle c_j \otimes c_i \rangle \\ \langle c_j^\dagger \otimes c_i^\dagger \rangle & \langle c_j \otimes c_i^\dagger \rangle \end{pmatrix} \quad (19)$$

$$\equiv \begin{pmatrix} \rho_{ee}^{ij} & \rho_{eh}^{ij} \\ \rho_{he}^{ij} & \rho_{hh}^{ij} \end{pmatrix} \equiv \begin{pmatrix} \rho_{ee}^{i\uparrow j\uparrow} & \rho_{ee}^{i\uparrow j\downarrow} & \rho_{eh}^{i\uparrow j\uparrow} & \rho_{eh}^{i\uparrow j\downarrow} \\ \rho_{ee}^{i\downarrow j\uparrow} & \rho_{ee}^{i\downarrow j\downarrow} & \rho_{eh}^{i\downarrow j\uparrow} & \rho_{eh}^{i\downarrow j\downarrow} \\ \rho_{he}^{i\uparrow j\uparrow} & \rho_{he}^{i\uparrow j\downarrow} & \rho_{hh}^{i\uparrow j\uparrow} & \rho_{hh}^{i\uparrow j\downarrow} \\ \rho_{he}^{i\downarrow j\uparrow} & \rho_{he}^{i\downarrow j\downarrow} & \rho_{hh}^{i\downarrow j\uparrow} & \rho_{hh}^{i\downarrow j\downarrow} \end{pmatrix}$$

and relating to themselves and to each other as

$$\rho_{ee}^{ij} = (\rho_{ee}^{ji})^\dagger \quad (20)$$

$$\rho_{eh}^{ij} = -(\rho_{eh}^{ji})^T \quad (21)$$

$$\rho_{hh}^{ij} = \delta_{ij} - (\rho_{ee}^{ji})^T \quad (22)$$

$$\rho_{he}^{ij} = (\rho_{eh}^{ji})^\dagger \quad (23)$$

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* $\mathbf{i} \equiv (i, s_i)$ does not underlies the objects spin structure, so beware the differences between $\rho_{ee}^{ij} = \rho_{ee}^{i s_i j s_j}$ and $\rho_{ee}^{ij} = [\rho_{ee}^{i\uparrow j\uparrow} \ \rho_{ee}^{i\uparrow j\downarrow}; \rho_{ee}^{i\downarrow j\uparrow} \ \rho_{ee}^{i\downarrow j\downarrow}]$. The notation ρ_{ee}^{ij} 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 $\check{\rho}^{ij} = [\rho_{ee}^{ij} \ \rho_{eh}^{ij}; \rho_{he}^{ij} \ \rho_{hh}^{ij}]$.

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

$$\frac{d}{dt} \rho_{ee}^{ij} = \frac{\iota}{\hbar} \langle [H, c_j^\dagger] c_i \rangle + \frac{i}{\hbar} \langle c_j^\dagger [H, c_i] \rangle \quad (24)$$

with H the Hamiltonian in Eq.(11) and ι 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,

$$[H, c_j^\dagger] = \sum_{\alpha\beta} H_0^{\alpha\beta} [c_\alpha^\dagger c_\beta, c_j^\dagger] + \frac{1}{2} \sum_{\alpha\beta} v^{\alpha\beta} [c_\alpha^\dagger c_\beta^\dagger c_\beta c_\alpha, c_j^\dagger]$$

$$[H, c_i] = \sum_{\alpha\beta} H_0^{\alpha\beta} [c_\alpha^\dagger c_\beta, c_i] + \frac{1}{2} \sum_{\alpha\beta} v^{\alpha\beta} [c_\alpha^\dagger c_\beta^\dagger c_\beta c_\alpha, c_i]$$

The commutators reading

$$[c_\alpha^\dagger c_\beta, c_j^\dagger] = c_\alpha^\dagger \delta_{\beta j} \quad (25)$$

$$[c_\alpha^\dagger c_\beta, c_i] = -c_\beta \delta_{i\alpha} \quad (26)$$

$$[c_\alpha^\dagger c_\beta^\dagger c_\beta c_\alpha, c_j^\dagger] = c_\alpha^\dagger c_\beta^\dagger c_\beta \delta_{\alpha j} - c_\alpha^\dagger c_\beta^\dagger c_\alpha \delta_{\beta j} \quad (27)$$

$$[c_\alpha^\dagger c_\beta^\dagger c_\beta c_\alpha, c_i] = c_\alpha^\dagger c_\beta c_\alpha \delta_{\beta i} - c_\beta^\dagger c_\beta c_\alpha \delta_{i\alpha} \quad (28)$$

where we used that

$$[AB, Z] = A\{B, Z\} - \{Z, A\}B \quad (29)$$

$$[ABCD, Z] = AB(C\{D, Z\} - \{Z, C\}D) + (A\{B, Z\} - \{Z, A\}B)CD \quad (30)$$

The complete Heisenberg commutators then yield

$$\begin{aligned} [H, c_j^\dagger] &= \sum_\alpha H_0^{\alpha j} c_\alpha^\dagger + \frac{1}{2} \sum_\beta v^{j\beta} c_j^\dagger c_\beta^\dagger c_\beta - \frac{1}{2} \sum_\alpha v^{\alpha j} c_\alpha^\dagger c_j^\dagger c_\alpha \\ &= \sum_\alpha H_0^{\alpha j} c_\alpha^\dagger + \frac{1}{2} \sum_\alpha v^{\alpha j} (c_j^\dagger c_\alpha^\dagger - c_\alpha^\dagger c_j^\dagger) c_\alpha \end{aligned} \quad (31)$$

$$\begin{aligned} [H, c_i] &= -\sum_\beta H_0^{i\beta} c_\beta + \frac{1}{2} \sum_\alpha v^{\alpha i} c_\alpha^\dagger c_i c_\alpha - \frac{1}{2} \sum_\beta v^{i\beta} c_\beta^\dagger c_\beta c_i \\ &= -\sum_\alpha H_0^{i\alpha} c_\alpha + \frac{1}{2} \sum_\alpha v^{\alpha i} c_\alpha^\dagger (c_i c_\alpha - c_\alpha c_i) \end{aligned} \quad (32)$$

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

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

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

$$\begin{aligned} i\hbar \frac{d}{dt} \rho_{ee}^{ij} &= -H_0^{\alpha j} \rho_{ee}^{i\alpha} + H_0^{i\alpha} \rho_{ee}^{\alpha j} \\ &- (v^{\alpha j} - v^{\alpha i}) \langle c_j^\dagger c_\alpha^\dagger c_\alpha c_i \rangle \end{aligned} \quad (33)$$

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

$$\langle c_j^\dagger c_\alpha^\dagger c_\alpha c_i \rangle \approx \rho_{he}^{\alpha j} \rho_{eh}^{i\alpha} - \rho_{ee}^{\alpha j} \rho_{ee}^{i\alpha} + \rho_{ee}^{ij} \rho_{ee}^{\alpha\alpha} \quad (34)$$

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

$$\Sigma_H^{ij} = \delta_{ij} \sum_\alpha v^{i\alpha} \rho_{ee}^{\alpha\alpha} \quad (35)$$

$$\Sigma_F^{ij} = -v^{ij} \rho_{ee}^{ij} \quad (36)$$

$$\Sigma_B^{ij} = v^{ij} \rho_{eh}^{ij} \quad (37)$$

The interacting term of Eq.(??) yield

$$\begin{aligned} &v^{\alpha j} \left[\rho_{he}^{\alpha j} \rho_{eh}^{i\alpha} - \rho_{ee}^{\alpha j} \rho_{ee}^{i\alpha} + \rho_{ee}^{ij} \rho_{ee}^{\alpha\alpha} \right] \\ &= \left\{ v^{\alpha j} \rho_{he}^{\alpha j} \right\} \rho_{eh}^{i\alpha} - \left\{ v^{\alpha j} \rho_{ee}^{\alpha j} \right\} \rho_{ee}^{i\alpha} + \rho_{ee}^{ij} \left\{ v^{\alpha j} \rho_{ee}^{\alpha\alpha} \right\} \\ &= \rho_{eh}^{i\alpha} \left(-\Sigma_B^{\alpha j} \right)^\dagger + \rho_{ee}^{i\alpha} \Sigma_F^{\alpha j} + \rho_{ee}^{ij} \Sigma_H^{ii} \\ &= \left[-\rho_{eh}^{ij} \left(-\Sigma_B^{ji} \right)^\dagger + \rho_{ee}^{ij} \Sigma_F^{ij} + \rho_{ee}^{ij} \Sigma_H^{ij} \delta_{ij} \right]^{s_i s_j} \quad (38) \\ &- v^{\alpha i} \left[\rho_{he}^{\alpha j} \rho_{eh}^{i\alpha} - \rho_{ee}^{\alpha j} \rho_{ee}^{i\alpha} + \rho_{ee}^{ij} \rho_{ee}^{\alpha\alpha} \right] \\ &= - \left(\rho_{he}^{\alpha j} \left\{ v^{i\alpha} \rho_{eh}^{i\alpha} \right\} + \rho_{ee}^{\alpha j} \left\{ -v^{i\alpha} \rho_{ee}^{i\alpha} \right\} + \rho_{ee}^{ij} \left\{ v^{i\alpha} \rho_{ee}^{\alpha\alpha} \right\} \right) \\ &= - \left(\Sigma_B^{i\alpha} \rho_{he}^{\alpha j} + \Sigma_F^{i\alpha} \rho_{ee}^{\alpha j} + \Sigma_H^{ii} \rho_{ee}^{ij} \right) \\ &= - \left[\Sigma_B^{ij} \rho_{he}^{ij} + \Sigma_F^{ij} \rho_{ee}^{ij} + \rho_{ee}^{ij} \Sigma_H^{ij} \delta_{ij} \right]^{s_i s_j} \quad (39) \end{aligned}$$

where $[\cdot]^{s_i s_j}$ is the element at position $s_i s_j$, e.g $[M]^\uparrow \uparrow = M[1, 1]$. 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),

$$\Sigma_B^{ij} = \left(v^{ij} \rho_{eh}^{ij} \right) = v^{ij} \left(-\rho_{eh}^{ji} \right) = -\Sigma_B^{ji} \quad (40)$$

$$\left(\Sigma_B^{ji} \right)^\dagger = \left(v^{ji} \rho_{eh}^{ji} \right)^\dagger = \left(v^{ij} \rho_{he}^{ij} \right) \stackrel{!}{=} - \left(\Sigma_B^{ij} \right)^\dagger \quad (41)$$

The purely electronic rDM EoM then yields

$$i\hbar \frac{d}{dt} \rho_{ee}^{ij} \approx \left[\mathbf{H}_{HF}^{ij}, \rho_{ee}^{ij} \right] + \Sigma_B^{ij} \cdot \rho_{he}^{ij} - \rho_{eh}^{ij} \cdot \left(\Sigma_B^{ji} \right)^\dagger \quad (42)$$

where we have defined

$$\mathbf{H}_{HF}^{ij} = \mathbf{H}_0^{ij} + \Sigma_H^{ij} \delta_{ij} + \Sigma_F^{ij} \quad (43)$$

Analogously for the anomalous rDM EoM, we obtain

$$\frac{d}{dt} \rho_{eh}^{ij} = \frac{i}{\hbar} \langle [H, c_j] c_i \rangle + \frac{i}{\hbar} \langle c_j [H, c_i] \rangle \quad (44)$$

$$\langle [H, c_j] c_i \rangle = - \sum_\alpha H_0^{j\alpha} \rho_{eh}^{i\alpha} - \sum_\alpha v^{\alpha j} \langle c_\alpha^\dagger c_\alpha c_j c_i \rangle \quad (45)$$

$$\langle c_j [H, c_i] \rangle = - \sum_\alpha H_0^{i\alpha} \rho_{eh}^{\alpha j} - \sum_\alpha v^{\alpha i} \langle c_j c_\alpha^\dagger c_\alpha c_i \rangle \quad (46)$$

$$\langle c_\alpha^\dagger c_\alpha c_j c_i \rangle \approx \rho_{ee}^{\alpha\alpha} \rho_{eh}^{ij} - \rho_{ee}^{j\alpha} \rho_{eh}^{i\alpha} + \rho_{ee}^{i\alpha} \rho_{eh}^{j\alpha} \quad (47)$$

$$\langle c_j c_\alpha^\dagger c_\alpha c_i \rangle \approx \rho_{hh}^{\alpha j} \rho_{eh}^{i\alpha} - \rho_{eh}^{\alpha j} \rho_{ee}^{i\alpha} + \rho_{eh}^{ij} \rho_{ee}^{\alpha\alpha} \quad (48)$$

and finally

$$\begin{aligned} i\hbar \frac{d}{dt} \rho_{eh}^{ij} \approx & \mathbf{H}_{HF}^{ij} \cdot \rho_{eh}^{ij} + \rho_{eh}^{ij} \cdot \left(\mathbf{H}_{HF}^{ij} \right)^T \\ & + \Sigma_B^{ij} \cdot \rho_{hh}^{ij} - \rho_{ee}^{ij} \cdot \Sigma_B^{ij} \end{aligned} \quad (49)$$

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

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

$$\check{H}_0^{ij} = \begin{pmatrix} \mathbf{H}_0^{ij} & 0 \\ 0 & -(\mathbf{H}_0^{ji})^T \end{pmatrix} \quad (51)$$

$$\check{\Sigma}^{ij} = \begin{pmatrix} \Sigma_H^{ij} + \Sigma_F^{ij} & \Sigma_B^{ij} \\ (\Sigma_B^{ji})^\dagger & -(\Sigma_H^{ji} + \Sigma_F^{ji})^T \end{pmatrix} \quad (52)$$

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

$$\begin{aligned} \Sigma_H^{ij} &= \delta_{ij} \sum_{\alpha} v^{i\alpha} \rho_{ee}^{\alpha\alpha} \\ &= \delta_{ij} \sigma_0 \sum_{\alpha} v^{i\alpha} \sum_{s_{\alpha}} \rho_{ee}^{\alpha s_{\alpha} \alpha s_{\alpha}} \\ &= \delta_{ij} \sigma_0 \sum_{\alpha} v^{i\alpha} (\rho_{ee}^{\alpha \uparrow \alpha \uparrow} + \rho_{ee}^{\alpha \downarrow \alpha \downarrow}) \\ &= \delta_{ij} \sigma_0 \sum_{\alpha} v^{i\alpha} \text{Tr}(\rho_{ee}^{\alpha\alpha}) \end{aligned} \quad (53)$$

$$= \delta_{ij} \sigma_0 \sum_{\alpha} v^{i\alpha} \left[\frac{1}{2} \text{Tr}([\tau_z \otimes \sigma_0] \check{\rho}^{\alpha\alpha}) + 1 \right] \quad (54)$$

$$\equiv \frac{1}{2} \delta_{ij} \sigma_0 \sum_{\alpha} v^{i\alpha} \text{Tr}([\tau_z \otimes \sigma_0] \check{\rho}^{\alpha\alpha}) \quad (55)$$

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

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

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

$$\Sigma_F^{ij} = -v^{ij} \rho_{ee}^{ij} \quad (57)$$

$$\Sigma_B^{ij} = v^{ij} \rho_{eh}^{ij} \quad (58)$$

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

rDM as

$$\begin{aligned} \Sigma_F^{ij} + \Sigma_B^{ij} &= -v^{ij} [\tau_z \otimes \sigma_0] \check{\rho}_{ij} [\tau_z \otimes \sigma_0] \\ &= -v^{ij} [\tau_z \otimes \sigma_0] \check{\rho}_{ij} [\tau_z \otimes \sigma_0] \end{aligned} \quad (59)$$

We can then compactly rewrite the Nambu mean field Hamiltonian as

$$\begin{aligned} \check{\Sigma}^{ij} &= \frac{1}{2} \delta_{ij} [\tau_z \otimes \sigma_0] \sum_{\alpha} v^{i\alpha} \text{Tr}([\tau_z \otimes \sigma_0] \check{\rho}^{\alpha\alpha}) \\ &\quad - v^{ij} [\tau_z \otimes \sigma_0] \check{\rho}^{ij} [\tau_z \otimes \sigma_0] \end{aligned} \quad (60)$$

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 $\Sigma_{H/F}^{ji} = \left(\Sigma_{H/F}^{ij} \right)^\dagger$ and the Bogoliubov term the symmetry from Eq.(21), i.e $\Sigma_B^{ij} = -\left(\Sigma_B^{ji} \right)^T$. From these constrains one can then see that

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

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

$$\begin{aligned} & \left(\begin{array}{cc} \left\{ \left[\Sigma_H^{ji} \right]^\dagger + \left[\Sigma_F^{ji} \right]^\dagger \right\}^* & \left\{ -\left[\Sigma_B^{ji} \right]^T \right\}^* \\ \left\{ \left(-\left[\Sigma_B^{ij} \right]^T \right)^\dagger \right\}^* & \left\{ -\left(\left[\Sigma_H^{ij} \right]^\dagger + \left[\Sigma_F^{ij} \right]^\dagger \right)^T \right\}^* \end{array} \right) \\ &= \begin{pmatrix} \left(\Sigma_H^{ji} + \Sigma_F^{ji} \right)^T & -\left(\Sigma_B^{ji} \right)^\dagger \\ -\Sigma_B^{ij} & -\left(\Sigma_H^{ij} + \Sigma_F^{ij} \right) \end{pmatrix} \end{aligned} \quad (62)$$

All these symmetries relations can be summarized as

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

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

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 $\check{Q} = [\tau_z \otimes \sigma_0]$. In this context, see that the potential as it is written Eq.(3) is no longer true, but should read instead as

$$V_{j'i'}^{ij} \approx Q_{s_i s_i'} v^{ij} Q_{s_j s_j'} \delta_{ii'} \delta_{jj'} \quad (65)$$

As intended, the spurious interaction

$$\frac{1}{2} \sum_{i s_i} \sum_{s_j'} \left(c_{i s_i}^\dagger Q^2 \Big|_{s_i s_j'} c_{i s_j'} \right) v^{ii} \quad (66)$$

cancel out when writing the Hamiltonian in its normal-ordered form leaving us only with

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

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

$$\Sigma_H^{ij} = \delta_{ij} Q \sum_{\alpha} v^{i\alpha} \text{Tr}(\rho_{ee}^{\alpha\alpha}) \quad (67)$$

$$\Sigma_F^{ij} = -v^{ij} Q \rho_{ee}^{ij} Q^T \quad (68)$$

$$\Sigma_B^{ij} = v^{ij} Q \rho_{eh}^{ij} Q^T \quad (69)$$

and thus, the Nambu self-energy becomes

$$\check{\Sigma}^{ij} = \frac{1}{2} \delta_{ij} \check{Q} \sum_{\alpha} v^{i\alpha} \text{Tr}(\check{Q} \check{\rho}^{\alpha\alpha}) - v^{ij} \check{Q} \check{\rho}^{ij} \check{Q} \quad (70)$$

1. Alternate Nambu basis

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

$$\bar{c}_i^\dagger = (c_i^\dagger \ [i\sigma_y c_i]) = (c_{i\uparrow}^\dagger \ c_{i\downarrow}^\dagger \ c_{i\downarrow} \ -c_{i\uparrow}) \quad (71)$$

These relate to the previous choice of basis as

$$\bar{c}_i = \bar{U} \check{c}_i \Leftrightarrow \check{c}_i = \bar{U}^\dagger \bar{c}_i \quad (72)$$

$$\bar{c}_i^\dagger = \check{c}_i^\dagger \bar{U}^\dagger \Leftrightarrow \check{c}_i^\dagger = \bar{c}_i^\dagger \bar{U} \quad (73)$$

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

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

The rotated basis Nambu rDMs, explicitly reading

$$\begin{aligned} \bar{\rho}_{ij} &= \langle \bar{c}_j^\dagger \otimes \bar{c}_i \rangle \\ &= \begin{pmatrix} \langle c_j^\dagger \otimes c_i \rangle & \langle [i\sigma_y c_j] \otimes c_i \rangle \\ \langle c_j^\dagger \otimes [i\sigma_y c_i]^\dagger \rangle & \langle [i\sigma_y c_j] \otimes [i\sigma_y c_i]^\dagger \rangle \end{pmatrix} \\ &= \begin{pmatrix} \rho_{ee}^{i\uparrow j\uparrow} & \rho_{ee}^{i\uparrow j\downarrow} & \rho_{eh}^{i\uparrow j\downarrow} & -\rho_{eh}^{i\uparrow j\uparrow} \\ \rho_{ee}^{i\downarrow j\uparrow} & \rho_{ee}^{i\downarrow j\downarrow} & \rho_{eh}^{i\downarrow j\downarrow} & -\rho_{eh}^{i\downarrow j\uparrow} \\ \rho_{he}^{i\downarrow j\uparrow} & \rho_{he}^{i\downarrow j\downarrow} & \rho_{hh}^{i\downarrow j\downarrow} & -\rho_{hh}^{i\downarrow j\uparrow} \\ -\rho_{he}^{i\uparrow j\uparrow} & -\rho_{he}^{i\uparrow j\downarrow} & -\rho_{hh}^{i\uparrow j\downarrow} & \rho_{hh}^{i\uparrow j\uparrow} \end{pmatrix} \end{aligned}$$

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

$$\bar{\rho}_{ij} = \langle \bar{c}_j^\dagger \otimes \bar{c}_i \rangle = \langle \check{c}_i^\dagger \bar{U}^\dagger \otimes \bar{U} \check{c}_i \rangle = \bar{U} \check{\rho}_{ij} \bar{U}^\dagger \quad (75)$$

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

$$\bar{\Sigma}^{ij} = \frac{1}{2} \delta_{ij} \bar{Q} \sum_{\alpha} v^{i\alpha} \text{Tr}(\bar{Q} \bar{\rho}^{\alpha\alpha}) - v^{ij} \bar{Q} \bar{\rho}^{ij} \bar{Q} \quad (76)$$

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

$$\text{Tr}(\bar{U}^\dagger \bar{Q} \bar{\rho}^{\alpha\alpha} \bar{U}) = \text{Tr}(\bar{U} \bar{U}^\dagger \bar{Q} \bar{\rho}^{\alpha\alpha}) = \text{Tr}(\bar{Q} \bar{\rho}^{\alpha\alpha}) \quad (77)$$

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

$$\bar{\Sigma}^{ij} = \begin{pmatrix} \Sigma_H^{ij} + \Sigma_F^{ij} & -i\Sigma_B^{ij} \sigma_y \\ (-i\Sigma_B^{ji} \sigma_y)^\dagger & -\sigma_y (\Sigma_H^{ji} + \Sigma_F^{ji})^T \sigma_y \end{pmatrix} \quad (78)$$

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

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

where

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

The Nambu symmetries relations for the rotated basis read as

$$\bar{\Sigma}^{ij} = (\bar{\Sigma}^{ji})^\dagger \quad (80)$$

$$\bar{\Sigma}^{ij} = -[\tau_y \otimes \sigma_y] (\bar{\Sigma}^{ij})^* [\tau_y \otimes \sigma_y] \quad (81)$$

D. Hubbard model

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

$$v^{ij} = U\delta_{ij} \quad (82)$$

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

$$\begin{aligned} H_{\text{int}} &= \frac{1}{2} \sum_{ij} c_i^\dagger c_i v^{ij} c_j^\dagger c_j - \frac{1}{2} \sum_i c_i^\dagger c_i v^{ii} \\ &= \frac{1}{2} \sum_{i s_i} \sum_{j s_j} c_{i s_i}^\dagger c_{i s_i} \{U\delta_{ij}\} c_{j s_j}^\dagger c_{j s_j} - \frac{1}{2} \sum_{i s_i} c_{i s_i}^\dagger c_{i s_i} \{U\delta_{ii}\} \\ &= \frac{1}{2} U \sum_{i s_i} \left[\left(c_{i s_i}^\dagger c_{i s_i} n_{i\uparrow} + c_{i s_i}^\dagger c_{i s_i} n_{i\downarrow} \right) - (n_{i\uparrow} + n_{i\downarrow}) \delta_{ii} \right] \\ &= \frac{1}{2} U \sum_i (n_{i\uparrow} n_{i\downarrow} + n_{i\downarrow} n_{i\uparrow}) \end{aligned} \quad (83)$$

where $n_{i s_i} = c_{i s_i}^\dagger c_{i s_i}$ is the number operator and

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

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

that

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

one can simply write

$$H_{\text{int}} \rightarrow H_U = U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (86)$$

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

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