A general Green function is given by:

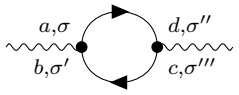
$$G_{ab}^{\sigma\sigma'}(i\omega_n) = \quad a,\sigma \longrightarrow b,\sigma' \tag{1}$$

Here $a$ and $b$ are spacial indices which would run from 0 to 1 in the case for the Hubbard dimer. In this case the Green function doesn't flip spin:

$$\delta_{\sigma\sigma'} G_{ab}^{\sigma\sigma'} = G_{ab}^{\sigma}(i\omega_n) = \quad a,\sigma \longrightarrow b,\sigma \tag{2}$$

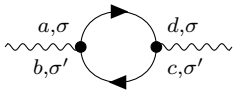
For the polarization we have:

$$P_{abcd}^{\sigma\sigma'\sigma''\sigma'''}(i\omega_n) = \tag{3}$$




But we know the Green functions don't change spin so we get:

$$\delta_{\sigma\sigma''}\delta_{\sigma'\sigma'''} P_{abcd}^{\sigma\sigma'\sigma''\sigma'''}(i\omega_n) = P_{abcd}^{\sigma\sigma'\sigma'\sigma}(i\omega_n) = P_{abcd}^{\sigma\sigma'}(i\omega_n) = \tag{4}$$

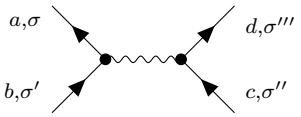



And in terms of the Green functions we have:

$$P_{abcd}^{\sigma\sigma'}(i\omega_n) = -\mathcal{F}_{\tau\to i\omega_n}\{G_{da}^{\sigma}(\tau)G_{bc}^{\sigma'}(-\tau)\}$$

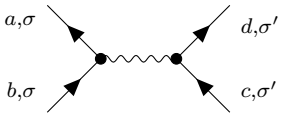
Note that the polarization is just the bubble diagram and without the Coulomb lines which would enforce additional restrictions as shown now. For the Coulomb interaction we have:

$$V_{abcd}^{\sigma\sigma'\sigma''\sigma'''} = \tag{5}$$




And if we say that the Coulomb interaction doesn't change spin we get:

$$\delta_{\sigma\sigma'}\delta_{\sigma''\sigma'''} V_{abcd}^{\sigma\sigma'\sigma''\sigma'''} = V_{abcd}^{\sigma\sigma\sigma''\sigma''} = V_{abcd}^{\sigma\sigma'} = \tag{6}$$




For the screened interaction we then get:

$$W_{abcd}^{\sigma\sigma'\sigma''\sigma'''}(i\omega_n) = V_{abcd}^{\sigma\sigma'\sigma''\sigma'''} + \sum_{\sigma_1\sigma_2\sigma_3\sigma_4}\sum_{abcd} V_{abef}^{\sigma\sigma'\sigma_3\sigma_4}\Pi_{fegh}^{\sigma_2\sigma_1\sigma_3\sigma_4}(i\omega_n)W_{hgcd}^{\sigma_4\sigma_3\sigma''\sigma'''}(i\omega_n) \tag{7}$$

$$= \delta_{\sigma\sigma'}\delta_{\sigma''\sigma'''}V_{abcd}^{\sigma\sigma'\sigma''\sigma'''} \tag{8}$$

$$+ \sum_{\sigma_1\sigma_2\sigma_3\sigma_4}\sum_{abcd}\delta_{\sigma\sigma'}\delta_{\sigma_3\sigma_4}V_{abef}^{\sigma\sigma'\sigma_3\sigma_4}\delta_{\sigma_2\sigma_3}\delta_{\sigma_1\sigma_4}\Pi_{fegh}^{\sigma_2\sigma_1\sigma_3\sigma_4}(i\omega_n)W_{hgcd}^{\sigma_4\sigma_3\sigma''\sigma'''}(i\omega_n) \tag{9}$$

$$= V_{abcd}^{\sigma\sigma\sigma''\sigma''} + \sum_{\sigma_1}\sum_{abcd} V_{abef}^{\sigma\sigma\sigma_1\sigma_1}\Pi_{fegh}^{\sigma_1\sigma_1\sigma_1\sigma_1}(i\omega_n)W_{hgcd}^{\sigma_1\sigma_1\sigma''\sigma'''}(i\omega_n) \tag{10}$$

$$W_{abcd}^{\sigma\sigma'}(i\omega_n) = V_{abcd}^{\sigma\sigma'} + \sum_{\sigma_1}\sum_{abcd} V_{abef}^{\sigma\sigma_1}\Pi_{fegh}^{\sigma_1}(i\omega_n)W_{hgcd}^{\sigma_1\sigma'}(i\omega_n) \tag{11}$$

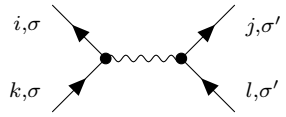
So in a spin full calculation, we have to explicitly sum over the spin when calculating the screened potential and if spin is not taken into account, the polarization diagram has a symmetry which results in a factor two. In our case with the Hubbard dimer, the two spin blocks are identical so we end up with this same factor of 2, explaining my earlier results. But this does raise the question on whether or not to include this factor for the Hartree contribution for the self energy. TPRF's GW solver doesn't take this into account so nor will I for comparison but this is something to think about.

For the Green function I'll use the following convention:

$$G_{ij}^{\sigma}(i\omega_n) = \quad i,\sigma \longrightarrow j,\sigma \tag{12}$$

Which carries only one spin index because we're only considering processes that don't flip the spin. For the Coulomb interaction I'll use the following convention:

$$V_{ijkl}^{\sigma\sigma'} = \tag{13}$$

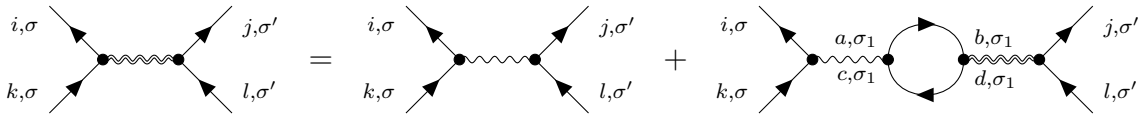



Which is consistent with:

$$\hat{V} = \frac{1}{2}\sum_{\sigma\sigma'}\sum_{ijkl} V_{ijkl}^{\sigma\sigma'}\hat{a}_{i\sigma}^{\dagger}\hat{a}_{j\sigma'}^{\dagger}\hat{a}_{l\sigma'}\hat{a}_{k\sigma} \tag{14}$$

For the screened interaction we have:

$$W_{ijkl}^{\sigma\sigma'} = \tag{15}$$



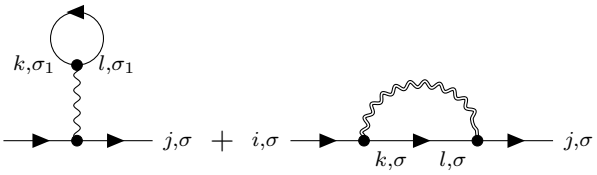

$$= V_{ijkl}^{\sigma\sigma'} + \sum_{\sigma_1}\sum_{abcd} V_{iakc}^{\sigma\sigma_1} P_{acbd}^{\sigma_1} W_{cjbl}^{\sigma_1\sigma'} \tag{16}$$

Where the polarization is now defined as:

$$P_{abcd}^{\sigma} \propto G_{ac}^{\sigma} G_{db}^{\sigma} \tag{17}$$

For the self energy we have:

$$\Sigma_{ij}^{\sigma} = \tag{18}$$




$$\propto \sum_{\sigma_1}\sum_{kl} V_{ljki}^{\sigma\sigma_1} G_{lk}^{\sigma_1} + W_{jkli}^{\sigma\sigma} G_{kl}^{\sigma} \tag{19}$$

Where the first term is the Hartree term and the second term can be split up into a dynamical part and the Fock term by splitting $W \to (W - V) + V$. And we can also see that for calculating the self energy, we only need the spin diagonal components of the screened potential.

Assuming the Coulomb interactions do not scatter, i.e. they don't change the position of an electron as well as preserve spin, we can instead write $V^{\sigma\sigma'}_{ijkl}$ as a two index object: $V^{\sigma\sigma'}_{ij} = V^{\sigma\sigma'}_{ijij}$, the same goes for $W$ and for $P$. This simplifies our equations to:

$$W^{\sigma\sigma'}_{ij} = V^{\sigma\sigma'}_{ij} + \sum_{\sigma_1,kl} V^{\sigma\sigma_1}_{ik} P^{\sigma_1}_{kl} W^{\sigma_1\sigma'}_{kj} \tag{20}$$

$$\tilde{\Sigma}^{\sigma}_{ij} = \tilde{W}^{\sigma\sigma}_{ij} G^{\sigma}_{ij} \tag{21}$$

$$\Sigma^{\sigma,\mathrm{Fock}}_{ij} = V^{\sigma\sigma}_{ij} G^{\sigma}_{ij} \tag{22}$$

$$\Sigma^{\sigma,\mathrm{Hartree}}_{ii} = \sum_{\sigma_1,j} V^{\sigma\sigma_1}_{ij} G^{\sigma_1}_{jj} \tag{23}$$