Slave-spin Hartee-Fock generalization to the multi-orbital case

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Let us assume that the DMFT's impurity Hamiltonian reads:

$$H = \sum_{a=1}^{N_{orb}} H_{ab} + \sum_{a=1}^{N_{orb}} \sum_{k\sigma}^{\epsilon_k<0} \frac{v_{1ak\sigma}}{\sqrt{V}} (d^\dagger_{a\sigma} c_{1ak\sigma} + H.c.) + \sum_{a=1}^{N_{orb}} \sum_{k\sigma}^{\epsilon_k<0} \frac{v_{2ak\sigma}}{\sqrt{V}} (d^\dagger_{a\sigma} c_{2ak\sigma} + H.c.) + H_{loc}(\{n_{a\sigma}\}),$$

where $H_b = \sum_{a=1}^{N_{orb}} \sum_{k\sigma}^{\epsilon_k<0} \vec{c}^\dagger_{ak\sigma} \sigma^x \vec{c}_{ak\sigma}$, N_{orb} number of orbitals and

$$\begin{cases} v_{1ak\sigma} & = (v_{ak\sigma} + v_{a\mathcal{C}_k\sigma})/\sqrt{2} \\ v_{2ak\sigma} & = (v_{ak\sigma} - v_{a\mathcal{C}_k\sigma})/\sqrt{2} \end{cases}, \quad \begin{cases} c_{1ak\sigma} & = (c_{ak\sigma} + c_{a\mathcal{C}_k\sigma})/\sqrt{2} \\ c_{2ak\sigma} & = (c_{ak\sigma} - c_{a\mathcal{C}_k\sigma})/\sqrt{2} \end{cases}. \tag{1}$$

On the Matsubara axis the unperturbed Green's function of the bath reads:

$$\hat{G}^0_{ak\sigma} = \begin{pmatrix} G^0_{11ak\sigma} & G^0_{12ak\sigma} \\ G^0_{21ak\sigma} & G^0_{22ak\sigma} \end{pmatrix} = \frac{1}{2}\left(\frac{1}{i\epsilon+\epsilon_k} + \frac{1}{i\epsilon-\epsilon_k}\right)\sigma^0 + \frac{1}{2}\left(\frac{1}{i\epsilon-\epsilon_k} - \frac{1}{i\epsilon+\epsilon_k}\right)\sigma^x.$$

The model can be exactly mapped without any constraint into the Hamiltonian (PRB 96, 201106(R)):

$$\begin{aligned} H_2 = & \sum_{a=1}^{N_{orb}} H_b + \sum_{a=1}^{N_{orb}} \sum_{\sigma} \tau^x_{a\sigma} T_{1a\sigma} + \sum_{\sigma} \tau^y_{a\sigma} J_{2a\sigma} \\ & + H_{loc}(\{\tau^z_{a\sigma}\}), \end{aligned}$$

where

$$T_{1a\sigma} = \sum_{k}^{\epsilon_k<0} \frac{v_{1ak\sigma}}{\sqrt{V}} (f^\dagger_{a\sigma} c_{1ak\sigma} + H.c.),$$

$$J_{2a\sigma} = i \sum_{k}^{\epsilon_k<0} \frac{v_{2ak\sigma}}{\sqrt{V}} (f^\dagger_{\sigma} c_{2ak\sigma} - H.c.),$$

and $H_{loc}(\{\tau^z_{a\sigma}\})$ is obtained from $H_{loc}(\{n_{a\sigma}\})$ by using the identity

$$n_{a\sigma} = \frac{1+\tau^z_{a\sigma}}{2}.$$

The mapping introduces $2 \times N_{orb}$ Ising variables $\tau^i_{a\sigma}$ that are coupled with a resonant level model through the hybridization $T_{1a\sigma}$ and the current operator $J_{2a\sigma}$. Mean-field decoupling gives rise to two coupled problems, an effective resonant level model:

$$H_f = \sum_{a=1}^{N_{orb}} H_{ab} + \sum_{\sigma a=1}^{N_{orb}} \langle \tau^x_{a\sigma} \rangle T_{1a\sigma} + \sum_{\sigma a=1}^{N_{orb}} \langle \tau^y_{a\sigma} \rangle J_{2a\sigma}, \tag{2}$$

and:

$$H_\sigma = H_{loc}(\{\tau^z_{a\sigma}\}) + \sum_{\sigma a=1}^{N_{orb}} \tau^x_{a\sigma} \langle T_{1a\sigma}\rangle + \sum_{\sigma a=1}^{N_{orb}} \tau^y_\sigma \langle J_{2a\sigma}\rangle. \tag{3}$$

To determine the mean-field effect of the fermions on Ising degrees of freedom we have to compute the f pseudofermion Green's function. We notice that, in Hamiltonian (2), the orbital index a is a conserved quantity and:

$$G^{-1}_{fa\sigma}(i\epsilon) = i\epsilon - \Sigma_{fa\sigma}(i\epsilon), \tag{4}$$

at mean-field level we have:

$$\Sigma_{fa\sigma}(i\epsilon) = \langle \tau^x_{a\sigma}\rangle^2 \Delta_{11a\sigma}(i\epsilon) + \langle \tau^y_{a\sigma}\rangle^2 \Delta_{22a\sigma}(i\epsilon), \tag{5}$$

where

$$\left(\Delta_{\alpha\beta}(i\epsilon)\right)_{a\sigma} = \int \frac{d\omega}{\pi} \frac{\left(\Gamma_{\alpha\beta}(\omega)\right)_{a\sigma}}{i\epsilon - \omega}, \tag{6}$$

and $\left(\Gamma_{\alpha\beta}(\omega)\right)_{a\sigma} = -\Im\left(\Delta_{\alpha\beta}(\omega)\right)_{a\sigma} = \pi\rho(\omega) v_{\alpha a\sigma}(\omega) v_{\beta a\sigma}(\omega)/2$. Before computing the fermionic averages let us write explicilty the relations between $\Gamma_{a\sigma}(\epsilon) = \pi\rho(\epsilon) v^2_{a\sigma}(\epsilon)$ and $\left(\Gamma_{a\sigma}(\omega)\right)_{\alpha\beta}$. Given the Weiss field:

$$\mathcal{G}_{a\sigma}(i\epsilon) = \frac{1}{i\epsilon - \Delta_{a\sigma}(i\epsilon)},$$

we define $\Gamma_{a\sigma}(\omega) = \Im \mathcal{G}^{R-1}_{a\sigma}(\omega)$ and

$$v_{1(2)a\sigma}(\epsilon) = \frac{\sqrt{\Gamma_{a\sigma}(\epsilon)} \pm \sqrt{\Gamma_{a\sigma}(-\epsilon)}}{\sqrt{2\pi\rho(\epsilon)}},$$

by using Eq. (1) we have

$$\Gamma_{11a\sigma}(\epsilon) = \frac{\left(\sqrt{\Gamma_{a\sigma}(\epsilon)} + \sqrt{\Gamma_{a\sigma}(-\epsilon)}\right)^2}{4}, \quad \Gamma_{22a\sigma}(\epsilon) = \frac{\left(\sqrt{\Gamma_{a\sigma}(\epsilon)} - \sqrt{\Gamma_{a\sigma}(-\epsilon)}\right)^2}{4}, \tag{7}$$

and

$$\Gamma_{12a\sigma}(\epsilon) = \frac{\Gamma_{a\sigma}(\epsilon) - \Gamma_{a\sigma}(-\epsilon)}{4} = \Gamma_{21a\sigma}(\epsilon), \tag{8}$$

see Fig. 2 for more details.

Symmetries; Let us consider the symmetries of the single particle propagators. From definitions Eqs. (7), (8) and (6) we obtain:

$$\Delta_{11a\sigma}(-i\epsilon) = -\Delta_{11a\sigma}(i\epsilon), \quad \Delta_{22a\sigma}(-i\epsilon) = -\Delta_{22a\sigma}(i\epsilon)$$

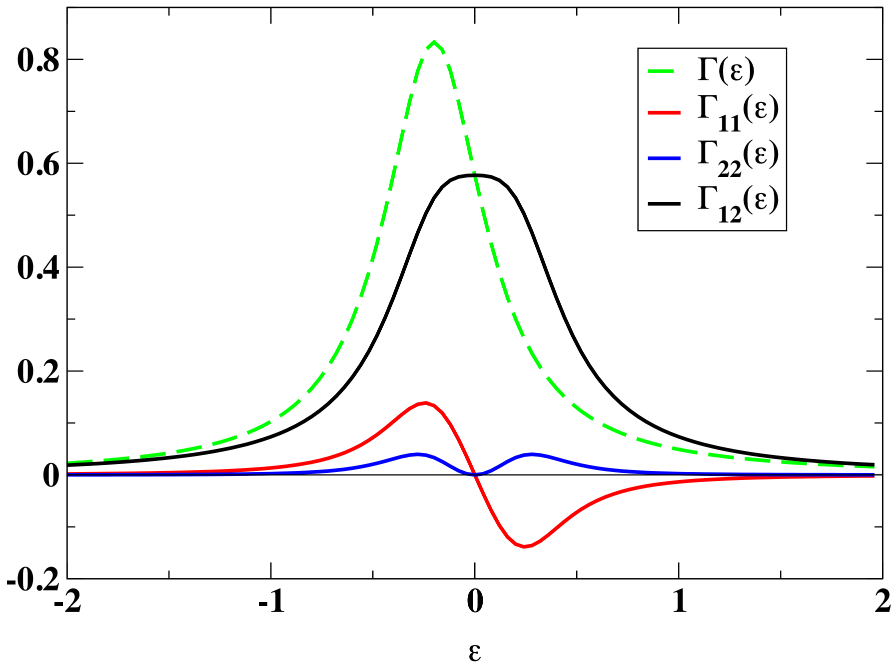

Figure 1: Decomposition of the original hybridization function in different compoenents.

and

$$\Delta_{12a\sigma}(-i\epsilon) = \Delta_{12a\sigma}(i\epsilon), \quad \Delta_{21a\sigma}(-i\epsilon) = \Delta_{21a\sigma}(i\epsilon).$$

Eqs. (4) and (5) implies:

$$G_{fa\sigma}(-i\epsilon) = -G_{fa\sigma}(i\epsilon),$$

i.e. the f pseudofermion spectral function is particle-hole symmetric $A_{fa\sigma}(\omega) = A_{fa\sigma}(-\omega)$.

Fermionic averages; Given the f pseudofermion we compute hybridization and current averages:

$$\begin{aligned}
\langle T_{1a\sigma}\rangle &= \frac{2}{\langle\tau^x_{a\sigma}\rangle} T \sum_{i\epsilon} \Sigma_{11a\sigma}(i\epsilon) G_{fa\sigma}(i\epsilon) \\
&= \frac{2}{\langle\tau^x_{a\sigma}\rangle\pi} \int dx \int dy A_{fa\sigma}(x) \langle\tau^x_{\sigma}\rangle^2 \Gamma_{11a\sigma}(y) \frac{f(x)-f(y)}{x-y}, \\
&= \frac{2\langle\tau^x_{a\sigma}\rangle}{\pi} \int dx \int dy \left[A_{fa\sigma}(x)\Gamma_{11a\sigma}(y) + A_{fa\sigma}(y)\Gamma_{11a\sigma}(x)\right] \frac{f(x)}{x-y},
\end{aligned}$$

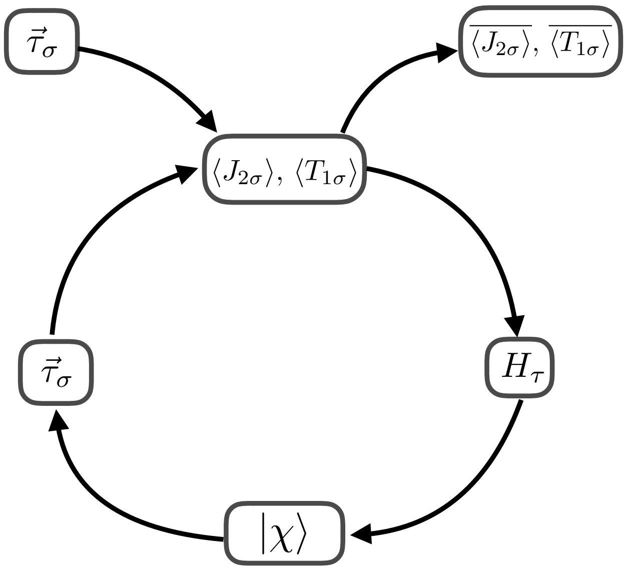

Figure 2: Schematic representation of the self consistent mean field loop to obtained the best factorised wave function. Convergence is reached when $\delta V_i = |(\langle T_{1\sigma}\rangle_{i+1} - \langle T_{1\sigma}\rangle_i, \langle J_{2\sigma}\rangle_{i+1} - \langle J_{2\sigma}\rangle_i)|$ is smaller than a given tolerance.

with $A_{f\sigma}(\epsilon) = -\Im G^R_{f\sigma}(\epsilon)/\pi$ and $f(x) = 1/(e^{\beta x}+1)$.

$$\begin{aligned}\langle J_{2a\sigma}\rangle &= \frac{2}{\langle \tau^y_{a\sigma}\rangle} T \sum_{i\epsilon} \Sigma_{22a\sigma}(i\epsilon) G_{fa\sigma}(i\epsilon) \\ &= \frac{2\langle \tau^y_{a\sigma}\rangle}{\pi} \int dx \int dy A_{fa\sigma}(x)\Gamma_{22a\sigma}(y) \frac{f(x)-f(y)}{x-y}, \\ &= \frac{2\langle \tau^y_{a\sigma}\rangle}{\pi} \int dx \int dy \left[A_{fa\sigma}(x)\Gamma_{22a\sigma}(y) + A_{fa\sigma}(y)\Gamma_{22a\sigma}(x)\right] \frac{f(x)}{x-y}.\end{aligned}$$

Given $\langle T_{1a\sigma}\rangle$ and $\langle J_{2a\sigma}\rangle$ we can obtain the spin Hamiltonian H_σ and its ground state $|\chi\rangle$, then we iterate the loop in Fig. 1 up to self consistency.

The single particle Green's function of the original fermions reads:

$$\begin{aligned}G_{da\sigma}(\tau) &= -2\langle T_\tau(\tau^-_{a\sigma}(\tau) f_{a\sigma}(\tau) \tau^+_{a\sigma} f^\dagger_{a\sigma})\rangle \\ &\simeq -2\langle T_\tau(\tau^-_{a\sigma}(\tau)\tau^+_{a\sigma})\rangle\langle T_\tau(f_{a\sigma}(\tau) f_{a\sigma})\rangle = -2G_{fa\sigma}(\tau)\Pi^\sigma_{-+a}(\tau),\end{aligned}$$

(the factor 2 follows from the slave-spin mapping) in Matsubara frequencies we have

$$G_{da\sigma}(i\epsilon)/2 = -T\sum_{i\omega} \Pi^\sigma_{-+a}(i\epsilon - i\omega) G_{fa\sigma}(i\epsilon).$$

From the previous equation follows the normalization condition on the real axis

$$\int A_{da\sigma}(\epsilon) d\epsilon = -\int \frac{d\omega}{\pi} \coth\frac{\beta\omega}{2} \Im\Pi^{\sigma R}_{-+a}(\omega) = \langle\{\tau^-_\sigma, \tau^+_\sigma\}\rangle = 1.$$

The bare spin correlation functions takes the general form:

$$\Pi^{\sigma}_{\alpha\beta a}(i\omega) = -\beta\delta(\Omega)\langle\chi|\tau^{\alpha}_{a\sigma}|\chi\rangle\langle\chi|\tau^{\beta}_{a\sigma}|\chi\rangle$$
$$+\sum_{n}^{n\neq 0}\left(\frac{\langle\chi|\tau^{\alpha}_{a\sigma}|\phi_n\rangle\langle\phi_n|\tau^{\beta}_{a\sigma}|\chi\rangle}{i\Omega-\omega_{n0}} - \frac{\langle\phi_n|\tau^{\alpha}_{a\sigma}|\chi\rangle\langle\chi|\tau^{\beta}_{a\sigma}|\phi_n\rangle}{i\Omega+\omega_{n0}}\right),$$

where $\omega_{n0} = E_n - E_0$, $|\chi\rangle$ is the two Ising variables ground state and $|\phi_n\rangle$ the excited configurations. Thus,

$$G_{da\sigma}(i\epsilon) = 2\langle\chi|\tau^{-}_{a\sigma}|\chi\rangle\langle\chi|\tau^{+}_{a\sigma}|\chi\rangle G_{fa\sigma}(i\epsilon) - 2T\sum_{i\omega}\tilde{\Pi}^{\sigma}_{-+a}(i\epsilon - i\omega)G_{fa\sigma}(i\omega),$$

where

$$\tilde{\Pi}^{\sigma}_{-+a}(i\Omega) = \int_0^{\beta} d\tau e^{i\Omega\tau}\tilde{\Pi}^{\sigma}_{-+a}(\tau).$$

The final result is:

$$A_{da\sigma}(\epsilon) = 2\langle\chi|\tau^{-}_{a\sigma}|\chi\rangle\langle\chi|\tau^{+}_{a\sigma}|\chi\rangle A_{fa\sigma}(\epsilon) + 2\int\frac{dx}{\pi}A_{fa\sigma}(\epsilon - x)\Im\tilde{\Pi}^{\sigma R}_{-+a}(x)\left(f(\epsilon - x) + n(-x)\right). \tag{9}$$

Neglecting RPA corrections;

$$\Im\tilde{\Pi}^{\sigma R}_{-+a}(x) = -\pi\sum_{n}^{n\neq 0}\delta(x-\omega_{n0})\langle\chi|\tau^{-}_{a\sigma}|\phi_n\rangle\langle\phi_n|\tau^{+}_{a\sigma}|\chi\rangle + \pi\sum_{n}^{n\neq 0}\delta(x+\omega_{n0})\langle\phi_n|\tau^{-}_{a\sigma}|\chi\rangle\langle\chi|\tau^{+}_{a\sigma}|\phi_n\rangle,$$

and

$$A_{da\sigma}(\epsilon) = 2\langle\chi|\tau^{-}_{a\sigma}|\chi\rangle\langle\chi|\tau^{+}_{a\sigma}|\chi\rangle A_{fa\sigma}(\epsilon)$$
$$+ 2\sum_{n>0}\theta(\epsilon - \omega_{n0})A_{fa\sigma}(\epsilon - \omega_{n0})\langle\chi|\tau^{-}_{a\sigma}|\phi_n\rangle\langle\phi_n|\tau^{+}_{a\sigma}|\chi\rangle$$
$$+ 2\sum_{n>0}\theta(-\epsilon - \omega_{n0})A_{fa\sigma}(\epsilon + \omega_{n0})\langle\phi_n|\tau^{-}_{a\sigma}|\chi\rangle\langle\chi|\tau^{+}_{a\sigma}|\phi_n\rangle.$$

Pauli principle implies

$$\int A_{da\sigma}(\epsilon)d\epsilon = 1,$$

and

$$\int A_{da\sigma}(\epsilon)d\epsilon = 2\langle\chi|\tau^{-}_{a\sigma}|\chi\rangle\langle\chi|\tau^{+}_{a\sigma}|\chi\rangle + \sum_{n>0}\langle\chi|\tau^{-}_{a\sigma}|\phi_n\rangle\langle\phi_n|\tau^{+}_{a\sigma}|\chi\rangle + \sum_{n>0}\langle\phi_n|\tau^{-}_{a\sigma}|\chi\rangle\langle\chi|\tau^{+}_{a\sigma}|\phi_n\rangle$$
$$= \langle\chi|\left\{\tau^{-}_{a\sigma}, \tau^{+}_{a\sigma}\right\}|\chi\rangle = 1.$$

RPA corrections; Diagrammatics calculations allow to derive the equations for the RPA spin correlation functions (dropping the orbital, spin indeces and the frequency dependence):

$$\begin{pmatrix} \Pi_{xx}^{-1}\left(1-\Pi_{xx}\chi_{T_1T_1}-\Pi_{xy}\chi_{J_2T_1}\right) & -\Pi_{xx}^{-1}\Pi_{xy}\chi_{J_2J_2}-\chi_{T_1J_2} \\ -\chi_{T_1T_1}-\Pi_{yx}^{-1}\Pi_{yy}\chi_{J_2T_1} & \Pi_{yx}^{-1}\left(1-\Pi_{yy}\chi_{J_2J_2}-\Pi_{yx}\chi_{T_1J_2}\right) \end{pmatrix}\cdot\begin{pmatrix} \overline{\Pi}_{xx} \\ \overline{\Pi}_{yx} \end{pmatrix}=\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{10}$$

$$\begin{pmatrix} \Pi_{xy}^{-1}\left(1-\Pi_{xx}\chi_{T_1T_1}-\Pi_{xy}\chi_{J_2T_1}\right) & -\chi_{J_2J_2}-\Pi_{xy}^{-1}\Pi_{xx}\chi_{T_1J_2} \\ -\Pi_{yy}^{-1}\Pi_{yx}\chi_{T_1T_1}-\chi_{J_2T_1} & \Pi_{yy}^{-1}\left(1-\Pi_{yy}\chi_{J_2J_2}-\Pi_{yx}\chi_{T_1J_2}\right) \end{pmatrix}\cdot\begin{pmatrix} \overline{\Pi}_{xy} \\ \overline{\Pi}_{yy} \end{pmatrix}=\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{11}$$

where

$$\chi_{T_1T_1}(\tau)=-\langle T_\tau(T_1(\tau)T_1)\rangle, \quad \chi_{J_2J_2}(\tau)=-\langle T_\tau(J_2(\tau)J_2)\rangle,$$

and

$$\chi_{T_1J_2}(\tau)=-\langle T_\tau(T_1(\tau)J_2)\rangle, \quad \chi_{J_2T_1}(\tau)=-\langle T_\tau(J_2(\tau)T_1)\rangle.$$

Given ω Eqs. (10) and (11) is algebraic problem:

$$\hat{K}(\omega)\cdot\vec{\Pi}(\omega)=\vec{1} \implies \vec{\Pi}(\omega)=\hat{K}^{-1}(\omega)\cdot\vec{1},$$

which can be solved analyticaly through:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \to \frac{1}{ad-bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}.$$

Finally, we obtain

$$\Pi_{-+}=\frac{\Pi_{xx}+\Pi_{yy}+i\Pi_{xy}-i\Pi_{yx}}{4},$$

that gives the incoherent part of the spectral function, second term on the right hand side of Eq. (9) . The following part of the paragraph is devoted to the evaluation of the self energy contributions. On the Matsubara axis we obtain (notice in the following $\sigma=(\sigma,a)$ encodes both the spin and the orbital degrees of freedom):

$$\begin{aligned}
\chi^{\sigma}_{T_1T_1}(i\Omega) = {} & 2T\sum_{i\epsilon}G_{f\sigma}(i\epsilon+i\Omega)G_{f\sigma}(i\epsilon)i\epsilon\left[\Delta_{11\sigma}(i\epsilon+i\Omega)+\Delta_{11\sigma}(i\epsilon)\right]-\langle T_{1\sigma}\rangle/\langle\tau^x_\sigma\rangle \\
& -2T\langle\tau^y_\sigma\rangle^2\sum_{i\epsilon}G_{f\sigma}(i\epsilon+i\Omega)G_{f\sigma}(i\epsilon)\Delta_{22\sigma}(i\epsilon)\left[\Delta_{11\sigma}(i\epsilon+i\Omega)+\Delta_{11\sigma}(i\epsilon)\right] \\
& -2T\langle\tau^y_\sigma\rangle^2\sum_{i\epsilon}G_{f\sigma}(i\epsilon+i\Omega)G_{f\sigma}(i\epsilon)\Delta_{12\sigma}(i\epsilon)\left[\Delta_{12\sigma}(i\epsilon+i\Omega)-\Delta_{12\sigma}(i\epsilon)\right],
\end{aligned}$$

and

$$
\begin{aligned}
\chi^{\sigma}_{J_2 J_2}(i\Omega) = 2T \sum_{i\epsilon} & G_{f\sigma}(i\epsilon + i\Omega) G_{f\sigma}(i\epsilon) i\epsilon \left[\Delta_{22\sigma}(i\epsilon + i\Omega) + \Delta_{22\sigma}(i\epsilon)\right] - \langle J_{2\sigma}\rangle / \langle \tau^y_\sigma \rangle \\
& - 2T \langle \tau^x_\sigma \rangle^2 \sum_{i\epsilon} G_{f\sigma}(i\epsilon + i\Omega) G_{f\sigma}(i\epsilon) \Delta_{11\sigma}(i\epsilon) \left[\Delta_{22\sigma}(i\epsilon + i\Omega) + \Delta_{22\sigma}(i\epsilon)\right] \\
& - 2T \langle \tau^x_\sigma \rangle^2 \sum_{i\epsilon} G_{f\sigma}(i\epsilon + i\Omega) G_{f\sigma}(i\epsilon) \Delta_{12\sigma}(i\epsilon) \left[\Delta_{12\sigma}(i\epsilon + i\Omega) - \Delta_{12\sigma}(i\epsilon)\right].
\end{aligned}
$$

Finally,

$$
\begin{aligned}
\chi^{\sigma}_{T_1 J_2}(i\Omega) = 2iT \sum_{i\epsilon} & G_{f\sigma}(i\epsilon + i\Omega) G_{f\sigma}(i\epsilon) \Delta_{12\sigma}(i\epsilon)(2i\epsilon + i\Omega) \\
& + 2T \langle \tau^y_\sigma \rangle \langle \tau^x_\sigma \rangle \sum_{i\epsilon} G_{f\sigma}(i\epsilon + i\Omega) G_{f\sigma}(i\epsilon) \Delta_{22\sigma}(i\epsilon) \left[\Delta_{11\sigma}(i\epsilon + i\Omega) + \Delta_{11\sigma}(i\epsilon)\right] \\
& + 2T \langle \tau^y_\sigma \rangle \langle \tau^x_\sigma \rangle \sum_{i\epsilon} G_{f\sigma}(i\epsilon + i\Omega) G_{f\sigma}(i\epsilon) \Delta_{12\sigma}(i\epsilon) \left[\Delta_{12\sigma}(i\epsilon + i\Omega) - \Delta_{12\sigma}(i\epsilon)\right],
\end{aligned}
$$

and

$$
\begin{aligned}
\chi^{\sigma}_{J_2 T_1}(i\Omega) = 2iT \sum_{i\epsilon} & G_{f\sigma}(i\epsilon + i\Omega) G_{f\sigma}(i\epsilon) \Delta_{12\sigma}(i\epsilon + i\Omega)(2i\epsilon + i\Omega) \\
& + 2T \langle \tau^y_\sigma \rangle \langle \tau^x_\sigma \rangle \sum_{i\epsilon} G_{f\sigma}(i\epsilon + i\Omega) G_{f\sigma}(i\epsilon) \Delta_{11\sigma}(i\epsilon) \left[\Delta_{22\sigma}(i\epsilon + i\Omega) + \Delta_{22\sigma}(i\epsilon)\right] \\
& + 2T \langle \tau^y_\sigma \rangle \langle \tau^x_\sigma \rangle \sum_{i\epsilon} G_{f\sigma}(i\epsilon + i\Omega) G_{f\sigma}(i\epsilon) \Delta_{12\sigma}(i\epsilon) \left[\Delta_{12\sigma}(i\epsilon + i\Omega) - \Delta_{12\sigma}(i\epsilon)\right].
\end{aligned}
$$