Lehmann representation of the one- and two-particle Green's function

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1 Lehmann representation of the Green's function

1.1 One-particle Green's function

On the real axis we want to obtain the retarded Green's function

$$G^R_{ab}(t,t') = -i\theta(t-t')\,\langle\{c_a(t)c^\dagger_b(t')\}\rangle \tag{1.1}$$

$$= -i\theta(t-t')\Big(\langle c_a(t)c^\dagger_b(t')\rangle - \langle c^\dagger_b(t')c_a(t)\rangle\,.\Big) \tag{1.2}$$

To obtain the Lehman representation we evaluate the first term and evaluate the expectation value using the Eigenbasis $|n\rangle$ of the Hamiltonian H

$$G^>_{ab}(t,t') = -i\,\langle c_a(t)c^\dagger_b(t')\rangle \tag{1.3}$$

$$= \frac{-i}{Z}\sum_n \mathrm{e}^{-\beta E_n}\,\langle n|\,\mathrm{e}^{iHt}c_a\mathrm{e}^{-iHt}\mathrm{e}^{iHt'}c^\dagger_b\mathrm{e}^{-iHt'}\,|n\rangle \tag{1.4}$$

$$= \frac{-i}{Z}\sum_{n,m} \mathrm{e}^{-\beta E_n}\,\langle n|\,\mathrm{e}^{iHt}c_a\mathrm{e}^{-iHt}\,|m\rangle\,\langle m|\,\mathrm{e}^{iHt'}c^\dagger_b\mathrm{e}^{-iHt'}\,|n\rangle \tag{1.5}$$

$$= \frac{-i}{Z}\sum_{n,m} \mathrm{e}^{-\beta E_n}\mathrm{e}^{i(E_n-E_m)(t-t')}\,\langle n|\,c_a\,|m\rangle\,\langle m|\,c^\dagger_b\,|n\rangle\,. \tag{1.6}$$

In the same way we get for the second term

$$
\begin{aligned}
G^{<}_{ab}(t,t') &= i\,\langle c^\dagger_b(t')c_a(t)\rangle && (1.7)\\
&= \frac{-i}{Z}\sum_{n,m} \mathrm{e}^{-\beta E_n}\mathrm{e}^{i(E_n-E_m)(t'-t)}\,\langle n|\,c^\dagger_b\,|m\rangle\,\langle m|\,c_a\,|n\rangle && (1.8)\\
&\overset{n\leftrightarrow m}{=} \frac{-i}{Z}\sum_{n,m} \mathrm{e}^{-\beta E_m}\mathrm{e}^{i(E_n-E_m)(t-t')}\,\langle n|\,c_a\,|m\rangle\,\langle m|\,c^\dagger_b\,|n\rangle\,. && (1.9)
\end{aligned}
$$

The full retarded Green's function is then given by

$$
G^R_{ab}(t-t') = \theta(t-t')\frac{-i}{Z}\sum_{n,m}\left(\mathrm{e}^{-\beta E_n}+\mathrm{e}^{-\beta E_m}\right)\mathrm{e}^{i(E_n-E_m)(t-t')}\,\langle n|\,c_a\,|m\rangle\,\langle m|\,c^\dagger_b\,|n\rangle\,. \tag{1.10}
$$

A Fourier transform to frequency space yields

$$
\begin{aligned}
G_{ab}(\omega) &= \int_{-\infty}^{\infty} G^R_{ab}(t)\mathrm{e}^{i(\omega+i\delta)t}\,\mathrm{d}t && (1.11)\\
&= \frac{-i}{Z}\sum_{n,m}\left(\mathrm{e}^{-\beta E_n}+\mathrm{e}^{-\beta E_m}\right)\langle n|\,c_a\,|m\rangle\,\langle m|\,c^\dagger_b\,|n\rangle\int_0^{\infty}\mathrm{e}^{i(w+i\delta+E_n-E_m)t}\,\mathrm{d}t && (1.12)\\
&= \frac{1}{Z}\sum_{n,m}\left(\mathrm{e}^{-\beta E_n}+\mathrm{e}^{-\beta E_m}\right)\frac{\langle n|\,c_a\,|m\rangle\,\langle m|\,c^\dagger_b\,|n\rangle}{w+i\delta+E_n-E_m}. && (1.13)
\end{aligned}
$$

The Matsubara Green's function is obtained by substituting $\omega+i\delta\to i\omega_n$.

We see that for a given $|n\rangle$ with N_n electrons, the summation over m can be restricted to the subspace with $N_m = N_n+1$ electrons, Or, respectively, for a given $|m\rangle$ with N_m electrons, the summation over n can be restricted to the subspace with $N_n = N_m - 1$ electrons.

1.2 Two-particle Green's function

We consider the two-particle Green's function $G^{(2)}_{\uparrow\downarrow}$ as defined in the PhD Thesis of G.Rohringer

$$
G^{(2)}_{\uparrow\downarrow}(\tau_1,\tau_2,\tau_3,\tau_4) = \langle T c^\dagger_\uparrow(\tau_1)c_\uparrow(\tau_2)c^\dagger_\downarrow(\tau_3)c_\downarrow(\tau_4)\rangle\,. \tag{1.14}
$$

The other spin combinations like $\uparrow\uparrow$ can by obtained from $G^{(2)}_{\uparrow\downarrow}$ by using symmetry relations.

Due to time-translational invariance we can set $\tau_4 = 0$, which leaves us with 6 distinct time orderings for τ_1, τ_2, τ_3

$$\begin{aligned} G^{(2)}_{\uparrow\downarrow}(\tau_1,\tau_2,\tau_3,\tau_4) = {} & \theta_{\tau_1>\tau_2>\tau_3} \langle c^\dagger_\uparrow(\tau_1) c_\uparrow(\tau_2) c^\dagger_\downarrow(\tau_3) c_\downarrow(0)\rangle \\ & - \theta_{\tau_1>\tau_3>\tau_2} \langle c^\dagger_\uparrow(\tau_1) c^\dagger_\downarrow(\tau_3) c_\uparrow(\tau_2) c_\downarrow(0)\rangle \\ & - \theta_{\tau_2>\tau_1>\tau_3} \langle c_\uparrow(\tau_2) c^\dagger_\uparrow(\tau_1) c^\dagger_\downarrow(\tau_3) c_\downarrow(0)\rangle \\ & + \theta_{\tau_2>\tau_3>\tau_1} \langle c_\uparrow(\tau_2) c^\dagger_\downarrow(\tau_3) c^\dagger_\uparrow(\tau_1) c_\downarrow(0)\rangle \\ & + \theta_{\tau_3>\tau_1>\tau_2} \langle c^\dagger_\downarrow(\tau_3) c^\dagger_\uparrow(\tau_1) c_\uparrow(\tau_2) c_\downarrow(0)\rangle \\ & - \theta_{\tau_3>\tau_2>\tau_1} \langle c^\dagger_\downarrow(\tau_3) c_\uparrow(\tau_2) c^\dagger_\uparrow(\tau_1) c_\downarrow(0)\rangle \end{aligned} \tag{1.15}$$

We now introduce the Eigenbasis $|m\rangle, |n\rangle, |o\rangle, |p\rangle$

$$\begin{aligned} \sum_{mnop} \mathrm{e}^{-\beta E_m} \Big(& + \theta_{\tau_1>\tau_2>\tau_3} \langle m|c^\dagger_\uparrow(\tau_1)|n\rangle \langle n|c_\uparrow(\tau_2)|o\rangle \langle o|c^\dagger_\downarrow(\tau_3)|p\rangle \langle p|c_\downarrow(0)|m\rangle \\ & - \theta_{\tau_1>\tau_3>\tau_2} \langle m|c^\dagger_\uparrow(\tau_1)|n\rangle \langle n|c^\dagger_\downarrow(\tau_3)|o\rangle \langle o|c_\uparrow(\tau_2)|p\rangle \langle p|c_\downarrow(0)|m\rangle \\ & - \theta_{\tau_2>\tau_1>\tau_3} \langle m|c_\uparrow(\tau_2)|n\rangle \langle n|c^\dagger_\uparrow(\tau_1)|o\rangle \langle o|c^\dagger_\downarrow(\tau_3)|p\rangle \langle p|c_\downarrow(0)|m\rangle \\ & + \theta_{\tau_2>\tau_3>\tau_1} \langle m|c_\uparrow(\tau_2)|n\rangle \langle n|c^\dagger_\downarrow(\tau_3)|o\rangle \langle o|c^\dagger_\uparrow(\tau_1)|p\rangle \langle p|c_\downarrow(0)|m\rangle \\ & + \theta_{\tau_3>\tau_1>\tau_2} \langle m|c^\dagger_\downarrow(\tau_3)|n\rangle \langle n|c^\dagger_\uparrow(\tau_1)|o\rangle \langle o|c_\uparrow(\tau_2)|p\rangle \langle p|c_\downarrow(0)|m\rangle \\ & - \theta_{\tau_3>\tau_2>\tau_1} \langle m|c^\dagger_\downarrow(\tau_3)|n\rangle \langle n|c_\uparrow(\tau_2)|o\rangle \langle o|c^\dagger_\uparrow(\tau_1)|p\rangle \langle p|c_\downarrow(0)|m\rangle \Big) \end{aligned} \tag{1.16}$$

$$\begin{aligned} = \sum_{mnop} \mathrm{e}^{-\beta E_m} \Big(& + \theta_{\tau_1>\tau_2>\tau_3} \mathrm{e}^{\tau_1(E_m-E_n)} \mathrm{e}^{\tau_2(E_n-E_o)} \mathrm{e}^{\tau_3(E_o-E_p)} \langle m|c^\dagger_\uparrow|n\rangle \langle n|c_\uparrow|o\rangle \langle o|c^\dagger_\downarrow|p\rangle \langle p|c_\downarrow|m\rangle \\ & - \theta_{\tau_1>\tau_3>\tau_2} \mathrm{e}^{\tau_1(E_m-E_n)} \mathrm{e}^{\tau_3(E_n-E_o)} \mathrm{e}^{\tau_2(E_o-E_p)} \langle m|c^\dagger_\uparrow|n\rangle \langle n|c^\dagger_\downarrow|o\rangle \langle o|c_\uparrow|p\rangle \langle p|c_\downarrow|m\rangle \\ & - \theta_{\tau_2>\tau_1>\tau_3} \mathrm{e}^{\tau_2(E_m-E_n)} \mathrm{e}^{\tau_1(E_n-E_o)} \mathrm{e}^{\tau_3(E_o-E_p)} \langle m|c_\uparrow|n\rangle \langle n|c^\dagger_\uparrow|o\rangle \langle o|c^\dagger_\downarrow|p\rangle \langle p|c_\downarrow|m\rangle \\ & + \theta_{\tau_2>\tau_3>\tau_1} \mathrm{e}^{\tau_2(E_m-E_n)} \mathrm{e}^{\tau_3(E_n-E_o)} \mathrm{e}^{\tau_1(E_o-E_p)} \langle m|c_\uparrow|n\rangle \langle n|c^\dagger_\downarrow|o\rangle \langle o|c^\dagger_\uparrow|p\rangle \langle p|c_\downarrow|m\rangle \\ & + \theta_{\tau_3>\tau_1>\tau_2} \mathrm{e}^{\tau_3(E_m-E_n)} \mathrm{e}^{\tau_1(E_n-E_o)} \mathrm{e}^{\tau_2(E_o-E_p)} \langle m|c^\dagger_\downarrow|n\rangle \langle n|c^\dagger_\uparrow|o\rangle \langle o|c_\uparrow|p\rangle \langle p|c_\downarrow|m\rangle \\ & - \theta_{\tau_3>\tau_2>\tau_1} \mathrm{e}^{\tau_3(E_m-E_n)} \mathrm{e}^{\tau_2(E_n-E_o)} \mathrm{e}^{\tau_1(E_o-E_p)} \langle m|c^\dagger_\downarrow|n\rangle \langle n|c_\uparrow|o\rangle \langle o|c^\dagger_\uparrow|p\rangle \langle p|c_\downarrow|m\rangle \Big). \end{aligned} \tag{1.17}$$

We now perform a Fourier transform $\tau_i \to i\omega_i$. The **first** term evaluates to

$$\int_0^\beta \mathrm{d}\tau_3 \mathrm{e}^{i\omega_3\tau_3} \int_0^\beta \mathrm{d}\tau_2 \mathrm{e}^{i\omega_2\tau_2} \int_0^\beta \mathrm{d}\tau_1 \mathrm{e}^{i\omega_1\tau_1} \Big(\mathrm{e}^{-\beta E_m} \theta_{\tau_1>\tau_2>\tau_3} \mathrm{e}^{\tau_1(E_m-E_n)} \mathrm{e}^{\tau_2(E_n-E_o)} \mathrm{e}^{\tau_3(E_o-E_p)} \Big) \tag{1.18}$$

$$= \mathrm{e}^{-\beta E_m} \int_0^\beta \mathrm{d}\tau_3 \mathrm{e}^{\tau_3(i\omega_3+E_o-E_p)} \int_{\tau_3}^\beta \mathrm{d}\tau_2 \mathrm{e}^{\tau_2(i\omega_2+E_n-E_o)} \int_{\tau_2}^\beta \mathrm{d}\tau_1 \mathrm{e}^{\tau_1(i\omega_1+E_m-E_n)} \tag{1.19}$$

$$= \mathrm{e}^{-\beta E_m} \int_0^\beta \mathrm{d}\tau_3 \mathrm{e}^{\tau_3(i\omega_3+E_o-E_p)} \int_{\tau_3}^\beta \mathrm{d}\tau_2 \mathrm{e}^{\tau_2(i\omega_2+E_n-E_o)} \frac{-\mathrm{e}^{\beta(E_m-E_n)} - \mathrm{e}^{\tau_2(i\omega_1+E_m-E_n)}}{i\omega_1+E_m-E_n} \tag{1.20}$$

$$= \frac{-1}{i\omega_1+E_m-E_n} \int_0^\beta \mathrm{d}\tau_3 \mathrm{e}^{\tau_3(i\omega_3+E_o-E_p)} \int_{\tau_3}^\beta \mathrm{d}\tau_2 \mathrm{e}^{\tau_2(i\omega_2+E_n-E_o)} \Big(\mathrm{e}^{-\beta E_n} + \mathrm{e}^{\tau_2(i\omega_1+E_m-E_n)} \mathrm{e}^{-\beta E_m} \Big) \tag{1.21}$$

$$\begin{aligned} = \frac{-1}{i\omega_1+E_m-E_n} \int_0^\beta \mathrm{d}\tau_3 \mathrm{e}^{\tau_3(i\omega_3+E_o-E_p)} \Big(& \mathrm{e}^{-\beta E_n} \frac{-\mathrm{e}^{\beta(E_n-E_o)} - \mathrm{e}^{\tau_3(i\omega_2+E_n-E_o)}}{i\omega_2+E_n-E_o} \\ & + \mathrm{e}^{-\beta E_m} \frac{+\mathrm{e}^{\beta(E_m-E_o)} - \mathrm{e}^{\tau_3(i\omega_1+i\omega_2+E_m-E_o)}}{i\omega_1+i\omega_2+E_m-E_o} \Big) \end{aligned} \tag{1.22}$$

$$\begin{aligned} = \frac{1}{i\omega_1+E_m-E_n} \int_0^\beta \mathrm{d}\tau_3 \mathrm{e}^{\tau_3(i\omega_3+E_o-E_p)} \Big(& \frac{\mathrm{e}^{-\beta E_o} + \mathrm{e}^{-\beta E_n} \mathrm{e}^{\tau_3(i\omega_2+E_n-E_o)}}{i\omega_2+E_n-E_o} \\ & - \frac{\mathrm{e}^{-\beta E_o} - \mathrm{e}^{-\beta E_m} \mathrm{e}^{\tau_3(i\omega_1+i\omega_2+E_m-E_o)}}{i\omega_1+i\omega_2+E_m-E_o} \Big) \end{aligned} \tag{1.23}$$

$$\begin{aligned} = \frac{1}{i\omega_1+E_m-E_n} \Big(& \frac{\int_0^\beta \mathrm{d}\tau_3 \mathrm{e}^{\tau_3(i\omega_3+E_o-E_p)}}{i\omega_2+E_n-E_o} \Big[\mathrm{e}^{-\beta E_o} + \mathrm{e}^{-\beta E_n} \mathrm{e}^{\tau_3(i\omega_2+E_n-E_o)} \Big] \\ & - \frac{\int_0^\beta \mathrm{d}\tau_3 \mathrm{e}^{\tau_3(i\omega_3+E_o-E_p)}}{i\omega_1+i\omega_2+E_m-E_o} \Big[\mathrm{e}^{-\beta E_o} - \mathrm{e}^{-\beta E_m} \mathrm{e}^{\tau_3(i\omega_1+i\omega_2+E_m-E_o)} \Big] \Big) \end{aligned} \tag{1.24}$$

$$\begin{aligned} = \frac{1}{i\omega_1+E_m-E_n} \Big(& \frac{1}{i\omega_2+E_n-E_o} \Big[\mathrm{e}^{-\beta E_o} \frac{-\mathrm{e}^{\beta(E_o-E_p)} - 1}{i\omega_3+E_o-E_p} + \mathrm{e}^{-\beta E_n} \frac{+\mathrm{e}^{\beta(E_n-E_p)} - 1}{i\omega_2+i\omega_3+E_n-E_p} \Big] \\ & - \frac{1}{i\omega_1+i\omega_2+E_m-E_o} \Big[\mathrm{e}^{-\beta E_o} \frac{-\mathrm{e}^{\beta(E_o-E_p)} - 1}{i\omega_3+E_o-E_p} - \mathrm{e}^{-\beta E_m} \frac{-\mathrm{e}^{\beta(E_m-E_p)} - 1}{i\omega_1+i\omega_2+i\omega_3+E_m-E_p} \Big] \Big) \end{aligned} \tag{1.25}$$

$$\begin{aligned} = \frac{1}{i\omega_1+E_m-E_n} \Big(& \frac{1}{i\omega_2+E_n-E_o} \Big[\frac{-\mathrm{e}^{-\beta E_p} - \mathrm{e}^{-\beta E_o}}{i\omega_3+E_o-E_p} + \frac{\mathrm{e}^{-\beta E_p} - \mathrm{e}^{-\beta E_n}}{i\omega_2+i\omega_3+E_n-E_p} \Big] \\ & - \frac{1}{i\omega_1+i\omega_2+E_m-E_o} \Big[\frac{-\mathrm{e}^{-\beta E_p} - \mathrm{e}^{-\beta E_o}}{i\omega_3+E_o-E_p} - \frac{-\mathrm{e}^{-\beta E_p} - \mathrm{e}^{-\beta E_m}}{i\omega_1+i\omega_2+i\omega_3+E_m-E_p} \Big] \Big) \end{aligned} \tag{1.26}$$

$$\begin{aligned} = \frac{-1}{i\omega_1+E_m-E_n} \Big(& \frac{1}{i\omega_2+E_n-E_o} \Big[\frac{\mathrm{e}^{-\beta E_o} + \mathrm{e}^{-\beta E_p}}{i\omega_3+E_o-E_p} + \frac{\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_p}}{i\omega_2+i\omega_3+E_n-E_p} \Big] \\ & - \frac{1}{i\omega_1+i\omega_2+E_m-E_o} \Big[\frac{\mathrm{e}^{-\beta E_o} + \mathrm{e}^{-\beta E_p}}{i\omega_3+E_o-E_p} - \frac{\mathrm{e}^{-\beta E_m} + \mathrm{e}^{-\beta E_p}}{i\omega_1+i\omega_2+i\omega_3+E_m-E_p} \Big] \Big). \end{aligned} \tag{1.27}$$

The **second** term evaluates to

$$- \int_0^\beta \mathrm{d}\tau_2 \mathrm{e}^{i\omega_2\tau_2} \int_0^\beta \mathrm{d}\tau_3 \mathrm{e}^{i\omega_3\tau_3} \int_0^\beta \mathrm{d}\tau_1 \mathrm{e}^{i\omega_1\tau_1} \Big(\mathrm{e}^{-\beta E_m} \theta_{\tau_1 > \tau_3 > \tau_2} \mathrm{e}^{\tau_1(E_m - E_n)} \mathrm{e}^{\tau_3(E_n - E_o)} \mathrm{e}^{\tau_2(E_o - E_p)} \Big) \tag{1.28}$$

$$= -\mathrm{e}^{-\beta E_m} \int_0^\beta \mathrm{d}\tau_2 \mathrm{e}^{\tau_2(i\omega_2 + E_o - E_p)} \int_0^\beta \mathrm{d}\tau_3 \mathrm{e}^{\tau_3(i\omega_3 + E_n - E_o)} \int_0^\beta \mathrm{d}\tau_1 \mathrm{e}^{\tau_1(i\omega_1 + E_m - E_n)}, \tag{1.29}$$

which we see is precisely the same expression as the first term, except we have to swap $i\omega_2 \leftrightarrow i\omega_3$, and flip the overall sign. Therefore, we get $f_{mnop}(\omega_1, \omega_3, \omega_2)$, where we have defined

$$\begin{aligned} f_{mnop}(\omega_1, \omega_2, \omega_3) = \frac{1}{i\omega_1 + E_m - E_n} \Big(& \frac{1}{i\omega_2 + E_n - E_o} \Big[\frac{\mathrm{e}^{-\beta E_o} + \mathrm{e}^{-\beta E_p}}{i\omega_3 + E_o - E_p} + \frac{\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_p}}{i\omega_2 + i\omega_3 + E_n - E_p} \Big] \\ & - \frac{1}{i\omega_1 + i\omega_2 + E_m - E_o} \Big[\frac{\mathrm{e}^{-\beta E_o} + \mathrm{e}^{-\beta E_p}}{i\omega_3 + E_o - E_p} - \frac{\mathrm{e}^{-\beta E_m} + \mathrm{e}^{-\beta E_p}}{i\omega_1 + i\omega_2 + i\omega_3 + E_m - E_p} \Big] \Big). \end{aligned} \tag{1.30}$$

For the **third** term we have to swap $i\omega_1 \leftrightarrow i\omega_2$ compared to the first term and obtain $f_{mnop}(\omega_2, \omega_1, \omega_3)$

For the **fourth** term we have to swap $i\omega_1 \leftrightarrow i\omega_3$ compared to the third term and obtain $-f_{mnop}(\omega_2, \omega_3, \omega_1)$

For the **fifth** term we have to swap $i\omega_2 \leftrightarrow i\omega_3$ compared to the third term and obtain $-f_{mnop}(\omega_3, \omega_1, \omega_2)$

For the **sixth** term we have to swap $i\omega_1 \leftrightarrow i\omega_2$ compared to the fifth term and obtain $f_{mnop}(\omega_3, \omega_2, \omega_1)$

Collecting all terms we obtain the final expression for the two-particle Green's function

$$\begin{aligned} G^{(2)}_{\uparrow\downarrow}(\omega_1, \omega_2, \omega_3) = \sum_{mnop} \Big(& - \langle m|c_\uparrow^\dagger|n\rangle \langle n|c_\uparrow|o\rangle \langle o|c_\downarrow^\dagger|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_1, \omega_2, \omega_3) \\ & + \langle m|c_\uparrow^\dagger|n\rangle \langle n|c_\downarrow^\dagger|o\rangle \langle o|c_\uparrow|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_1, \omega_3, \omega_2) \\ & + \langle m|c_\uparrow|n\rangle \langle n|c_\uparrow^\dagger|o\rangle \langle o|c_\downarrow^\dagger|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_2, \omega_1, \omega_3) \\ & - \langle m|c_\uparrow|n\rangle \langle n|c_\downarrow^\dagger|o\rangle \langle o|c_\uparrow^\dagger|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_2, \omega_3, \omega_1) \\ & - \langle m|c_\downarrow^\dagger|n\rangle \langle n|c_\uparrow^\dagger|o\rangle \langle o|c_\uparrow|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_3, \omega_1, \omega_2) \\ & + \langle m|c_\downarrow^\dagger|n\rangle \langle n|c_\uparrow|o\rangle \langle o|c_\uparrow^\dagger|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_3, \omega_2, \omega_1) \end{aligned} \tag{1.31}$$

When analyzing the overlap elements we see that each term corresponds to the following transitions: Starting with $|m\rangle$ being a state $m(N,S)$ with electron number

N and total spin S we get by going from right to left

$$\begin{aligned}
&(1): \ m(N,S) \to p(N-1,S+1) \to o(N,S) && \to n(N-1,S-1) \to m(N,S) \\
&(2): \ m(N,S) \to p(N-1,S+1) \to o(N-2,S) && \to n(N-1,S-1) \to m(N,S) \\
&(3): \ m(N,S) \to p(N-1,S+1) \to o(N,S) && \to n(N+1,S+1) \to m(N,S) \\
&(4): \ m(N,S) \to p(N-1,S+1) \to o(N,S+2) && \to n(N+1,S+1) \to m(N,S) \\
&(5): \ m(N,S) \to p(N-1,S+1) \to o(N-2,S) && \to n(N-1,S+1) \to m(N,S) \\
&(6): \ m(N,S) \to p(N-1,S+1) \to o(N,S+2) && \to n(N-1,S+1) \to m(N,S)
\end{aligned} \tag{1.32}$$

So we rearrange the terms grouping them by similar transitions in order to reuse results as much as possible in the code

$$\begin{aligned}
&(1): \ m(N,S) \to p(N-1,S+1) \to o(N,S) && \to n(N-1,S-1) \to m(N,S) \\
&(3): \ m(N,S) \to p(N-1,S+1) \to o(N,S) && \to n(N+1,S+1) \to m(N,S) \\
&(4): \ m(N,S) \to p(N-1,S+1) \to o(N,S+2) && \to n(N+1,S+1) \to m(N,S) \\
&(6): \ m(N,S) \to p(N-1,S+1) \to o(N,S+2) && \to n(N-1,S+1) \to m(N,S) \\
&(2): \ m(N,S) \to p(N-1,S+1) \to o(N-2,S) && \to n(N-1,S-1) \to m(N,S) \\
&(5): \ m(N,S) \to p(N-1,S+1) \to o(N-2,S) && \to n(N-1,S+1) \to m(N,S)
\end{aligned} \tag{1.33}$$

which results in

$$\begin{aligned}
G^{(2)}_{\uparrow\downarrow}(\omega_1,\omega_2,\omega_3) = \sum_{mnop} \Big(&- \langle m|c^\dagger_\uparrow|n\rangle \langle n|c_\uparrow|o\rangle \langle o|c^\dagger_\downarrow|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_1,\omega_2,\omega_3) \\
&+ \langle m|c_\uparrow|n\rangle \langle n|c^\dagger_\uparrow|o\rangle \langle o|c^\dagger_\downarrow|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_2,\omega_1,\omega_3) \\
&- \langle m|c_\uparrow|n\rangle \langle n|c^\dagger_\downarrow|o\rangle \langle o|c^\dagger_\uparrow|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_2,\omega_3,\omega_1) \\
&+ \langle m|c^\dagger_\downarrow|n\rangle \langle n|c_\uparrow|o\rangle \langle o|c^\dagger_\uparrow|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_3,\omega_2,\omega_1) \\
&+ \langle m|c^\dagger_\uparrow|n\rangle \langle n|c^\dagger_\downarrow|o\rangle \langle o|c_\uparrow|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_1,\omega_3,\omega_2) \\
&- \langle m|c^\dagger_\downarrow|n\rangle \langle n|c^\dagger_\uparrow|o\rangle \langle o|c_\uparrow|p\rangle \langle p|c_\downarrow|m\rangle f_{mnop}(\omega_3,\omega_1,\omega_2) \Big)
\end{aligned} \tag{1.34}$$

$$\begin{aligned}
= \sum_{mnop} \Big(&\big[- f_{mnop}(\omega_1,\omega_2,\omega_3) \langle m|c^\dagger_\uparrow|n\rangle \langle n|c_\uparrow|o\rangle + f_{mnop}(\omega_2,\omega_1,\omega_3) \langle m|c_\uparrow|n\rangle \langle n|c^\dagger_\uparrow|o\rangle \big] \langle o|c^\dagger_\downarrow|p\rangle \\
&\big[- f_{mnop}(\omega_2,\omega_3,\omega_1) \langle m|c_\uparrow|n\rangle \langle n|c^\dagger_\downarrow|o\rangle + f_{mnop}(\omega_3,\omega_2,\omega_1) \langle m|c^\dagger_\downarrow|n\rangle \langle n|c_\uparrow|o\rangle \big] \langle o|c^\dagger_\uparrow|p\rangle \\
&\big[+ f_{mnop}(\omega_1,\omega_3,\omega_2) \langle m|c^\dagger_\uparrow|n\rangle \langle n|c^\dagger_\downarrow|o\rangle - f_{mnop}(\omega_3,\omega_1,\omega_2) \langle m|c^\dagger_\downarrow|n\rangle \langle n|c^\dagger_\uparrow|o\rangle \big] \langle o|c_\uparrow|p\rangle \Big) \langle p|c_\downarrow|m\rangle
\end{aligned} \tag{1.35}$$

$$\tag{1.36}$$

Defining $f^{ijk}_{mnop} := f_{mnop}(\omega_i,\omega_j,\omega_k)$ and $c^1 := c^\dagger_\uparrow, c^2 := c_\uparrow, c^3 := c^\dagger_\downarrow$ and the overlap

$c^i_{mn} := \langle m|c_i|n\rangle$ this expression can be written as

$$\begin{aligned}
G^{(2),123}_{\uparrow\downarrow} &= -\sum_{mp}\Bigg[\sum_o\left(\sum_n f^{123}_{mnop}c^1_{mn}c^2_{no} - f^{213}_{mnop}c^2_{mn}c^1_{no}\right)c^3_{op} \\
&\qquad + \sum_o\left(\sum_n f^{231}_{mnop}c^2_{mn}c^3_{no} - f^{321}_{mnop}c^3_{mn}c^2_{no}\right)c^1_{op} \\
&\qquad + \sum_o\left(\sum_n f^{312}_{mnop}c^3_{mn}c^1_{no} - f^{132}_{mnop}c^1_{mn}c^3_{no}\right)c^2_{op}\Bigg]c^4_{pm} \qquad (1.37) \\
&= -\sum_{mp} g_{mp}c^4_{pm}, \qquad (1.38)
\end{aligned}$$

where

$$g_{mp} = g^{123}_{mp} + g^{231}_{mp} + g^{312}_{mp} \qquad (1.39)$$

$$g^{ijk}_{mp} = \sum_o g^{ij,k,sym}_{mop}c^k_{op} \qquad (1.40)$$

$$g^{ij,k,sym}_{mop} = g^{ij,k}_{mop} - g^{ji,k}_{mop} \qquad (1.41)$$

$$g^{ij,k}_{mop} = \sum_n f^{ijk}_{mnop}c^i_{mn}c^j_{no} \qquad (1.42)$$