# Lehmann representation of the oneand 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

$$G_{ab}^{R}(t,t') = -i\theta(t-t') \left\langle \left\{ c_a(t)c_b^{\dagger}(t') \right\} \right\rangle \tag{1.1}$$

$$= -i\theta(t - t') \left( \langle c_a(t)c_b^{\dagger}(t') \rangle - \langle c_b^{\dagger}(t')c_a(t) \rangle . \right)$$
 (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

$$G_{ab}^{>}(t,t') = -i \langle c_a(t)c_b^{\dagger}(t')\rangle \tag{1.3}$$

$$= \frac{-i}{Z} \sum_{n} e^{-\beta E_n} \langle n | e^{iHt} c_a e^{-iHt} e^{iHt'} c_b^{\dagger} e^{-iHt'} | n \rangle$$
 (1.4)

$$= \frac{-i}{Z} \sum_{n,m} e^{-\beta E_n} \langle n | e^{iHt} c_a e^{-iHt} | m \rangle \langle m | e^{iHt'} c_b^{\dagger} e^{-iHt'} | n \rangle$$
 (1.5)

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

In the same way we get for the second term

$$G_{ab}^{\leq}(t,t') = i \left\langle c_b^{\dagger}(t')c_a(t) \right\rangle \tag{1.7}$$

$$= \frac{-i}{Z} \sum_{n,m} e^{-\beta E_n} e^{i(E_n - E_m)(t' - t)} \langle n | c_b^{\dagger} | m \rangle \langle m | c_a | n \rangle$$
 (1.8)

$$\stackrel{n \leftrightarrow m}{=} \frac{-i}{Z} \sum_{n,m} e^{-\beta E_m} e^{i(E_n - E_m)(t - t')} \langle n | c_a | m \rangle \langle m | c_b^{\dagger} | n \rangle.$$
 (1.9)

The full retarded Green's function is then given by

$$G_{ab}^{R}(t-t') = \theta(t-t')\frac{-i}{Z}\sum_{n,m} \left(e^{-\beta E_n} + e^{-\beta E_m}\right) e^{i(E_n - E_m)(t-t')} \langle n|c_a|m\rangle \langle m|c_b^{\dagger}|n\rangle.$$

$$(1.10)$$

A Fourier transform to frequency space yields

$$G_{ab}(\omega) = \int_{-\infty}^{\infty} G_{ab}^{R}(t) e^{i(\omega + i\delta)t} dt$$
(1.11)

$$= \frac{-i}{Z} \sum_{n,m} \left( e^{-\beta E_n} + e^{-\beta E_m} \right) \langle n | c_a | m \rangle \langle m | c_b^{\dagger} | n \rangle \int_0^{\infty} e^{i(w+i\delta + E_n - E_m)t} dt \quad (1.12)$$

$$= \frac{1}{Z} \sum_{n,m} \left( e^{-\beta E_n} + e^{-\beta E_m} \right) \frac{\langle n | c_a | m \rangle \langle m | c_b^{\dagger} | n \rangle}{w + i\delta + E_n - E_m}.$$
 (1.13)

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

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  $G_{\uparrow\downarrow}^{(2)}$  as defined in the PhD Thesis of G.Rohringer

$$G_{\uparrow\downarrow}^{(2)}(\tau_1, \tau_2, \tau_3, \tau_4) = \langle T c_{\uparrow}^{\dagger}(\tau_1) c_{\uparrow}(\tau_2) c_{\downarrow}^{\dagger}(\tau_3) c_{\downarrow}(\tau_4) \rangle. \tag{1.14}$$

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

Due to time-translational invariance we can set  $\tau_4 = 0$ , which leaves us with 6

distinct time orderings for  $\tau_1, \tau_2, \tau_3$ 

$$G_{\uparrow\downarrow}^{(2)}(\tau_{1},\tau_{2},\tau_{3},\tau_{4}) = \theta_{\tau_{1}>\tau_{2}>\tau_{3}} \left\langle c_{\uparrow}^{\dagger}(\tau_{1})c_{\uparrow}(\tau_{2})c_{\downarrow}^{\dagger}(\tau_{3})c_{\downarrow}(0) \right\rangle$$

$$-\theta_{\tau_{1}>\tau_{3}>\tau_{2}} \left\langle c_{\uparrow}^{\dagger}(\tau_{1})c_{\downarrow}^{\dagger}(\tau_{3})c_{\uparrow}(\tau_{2})c_{\downarrow}(0) \right\rangle$$

$$-\theta_{\tau_{2}>\tau_{1}>\tau_{3}} \left\langle c_{\uparrow}(\tau_{2})c_{\uparrow}^{\dagger}(\tau_{1})c_{\downarrow}^{\dagger}(\tau_{3})c_{\downarrow}(0) \right\rangle$$

$$+\theta_{\tau_{2}>\tau_{3}>\tau_{1}} \left\langle c_{\uparrow}(\tau_{2})c_{\downarrow}^{\dagger}(\tau_{3})c_{\uparrow}^{\dagger}(\tau_{1})c_{\downarrow}(0) \right\rangle$$

$$+\theta_{\tau_{3}>\tau_{1}>\tau_{2}} \left\langle c_{\downarrow}^{\dagger}(\tau_{3})c_{\uparrow}^{\dagger}(\tau_{1})c_{\uparrow}(\tau_{2})c_{\downarrow}(0) \right\rangle$$

$$-\theta_{\tau_{3}>\tau_{2}>\tau_{1}} \left\langle c_{\downarrow}^{\dagger}(\tau_{3})c_{\uparrow}(\tau_{2})c_{\uparrow}^{\dagger}(\tau_{1})c_{\downarrow}(0) \right\rangle$$

$$(1.15)$$

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

$$\begin{split} \sum_{mnop} \mathrm{e}^{-\beta E_m} \Big( + \theta_{\tau_1 > \tau_2 > \tau_3} \left\langle m | c_\uparrow^\dagger(\tau_1) | n \right\rangle \left\langle n | c_\uparrow(\tau_2) | o \right\rangle \left\langle o | c_\downarrow^\dagger(\tau_3) | p \right\rangle \left\langle p | c_\downarrow(0) | m \right\rangle \\ - \theta_{\tau_1 > \tau_3 > \tau_2} \left\langle m | c_\uparrow^\dagger(\tau_1) | n \right\rangle \left\langle n | c_\downarrow^\dagger(\tau_3) | o \right\rangle \left\langle o | c_\uparrow(\tau_2) | p \right\rangle \left\langle p | c_\downarrow(0) | m \right\rangle \\ - \theta_{\tau_2 > \tau_1 > \tau_3} \left\langle m | c_\uparrow(\tau_2) | n \right\rangle \left\langle n | c_\uparrow^\dagger(\tau_1) | o \right\rangle \left\langle o | c_\downarrow^\dagger(\tau_3) | p \right\rangle \left\langle p | c_\downarrow(0) | m \right\rangle \\ + \theta_{\tau_2 > \tau_3 > \tau_1} \left\langle m | c_\uparrow(\tau_2) | n \right\rangle \left\langle n | c_\downarrow^\dagger(\tau_3) | o \right\rangle \left\langle o | c_\uparrow^\dagger(\tau_1) | p \right\rangle \left\langle p | c_\downarrow(0) | m \right\rangle \\ + \theta_{\tau_3 > \tau_1 > \tau_2} \left\langle m | c_\uparrow^\dagger(\tau_3) | n \right\rangle \left\langle n | c_\uparrow^\dagger(\tau_1) | o \right\rangle \left\langle o | c_\uparrow(\tau_2) | p \right\rangle \left\langle p | c_\downarrow(0) | m \right\rangle \\ - \theta_{\tau_3 > \tau_2 > \tau_1} \left\langle m | c_\downarrow^\dagger(\tau_3) | n \right\rangle \left\langle n | c_\uparrow(\tau_2) | o \right\rangle \left\langle o | c_\uparrow^\dagger(\tau_1) | p \right\rangle \left\langle p | c_\downarrow(0) | m \right\rangle \Big) \quad (1.16) \end{split}$$

$$= \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)} \left\langle m | c_\uparrow^\dagger | n \right\rangle \left\langle n | c_\uparrow | o \right\rangle \left\langle o | c_\downarrow^\dagger | p \right\rangle \left\langle p | c_\downarrow | m \right\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_3 (E_o - E_p)} \left\langle m | c_\uparrow | n \right\rangle \left\langle n | c_\uparrow^\dagger | o \right\rangle \left\langle o | c_\uparrow^\dagger | p \right\rangle \left\langle p | c_\downarrow | m \right\rangle \\ - \theta_{\tau_2 > \tau_1 > \tau_3} \mathrm{e}^{\tau_2 (E_m - E_n)} \mathrm{e}^{\tau_3 (E_n - E_o)} \mathrm{e}^{\tau_1 (E_o - E_p)} \left\langle m | c_\uparrow | n \right\rangle \left\langle n | c_\uparrow^\dagger | o \right\rangle \left\langle o | c_\uparrow^\dagger | p \right\rangle \left\langle p | c_\downarrow | m \right\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)} \left\langle m | c_\uparrow | n \right\rangle \left\langle n | c_\uparrow^\dagger | o \right\rangle \left\langle o | c_\uparrow^\dagger | p \right\rangle \left\langle p | c_\downarrow | m \right\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)} \left\langle m | c_\downarrow^\dagger | n \right\rangle \left\langle n | c_\uparrow^\dagger | o \right\rangle \left\langle o | c_\uparrow^\dagger | p \right\rangle \left\langle p | c_\downarrow | m \right\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)} \left\langle m | c_\downarrow^\dagger | n \right\rangle \left\langle n | c_\uparrow^\dagger | o \right\rangle \left\langle o | c_\uparrow^\dagger | p \right\rangle \left\langle p | c_\downarrow | m \right\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)} \left\langle m | c_\downarrow^\dagger | n \right\rangle \left\langle n | c_\uparrow^\dagger | o \right\rangle \left\langle o | c_\uparrow^\dagger | p \right\rangle \left\langle p | c_\downarrow | m \right\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$$

We now perform a Fourier transform  $\tau_i \to i\omega_i$ . The <u>first</u> term evaluates to

$$\begin{split} & \int_{0}^{\beta} \mathrm{d}\tau_{3} \mathrm{e}^{\omega_{3}\tau_{3}} \int_{0}^{\beta} \mathrm{d}\tau_{2} \mathrm{e}^{\omega_{2}\tau_{2}} \int_{0}^{\beta} \mathrm{d}\tau_{1} \mathrm{e}^{\omega_{2}\tau_{1}} \left( \mathrm{e}^{-\beta E_{m}} \theta_{\tau_{1} > \tau_{2} > \tau_{3}} \mathrm{e}^{\tau_{1}(E_{m} - E_{m})} \mathrm{e}^{\tau_{2}(E_{m} - E_{m})} \mathrm{e}^{\tau_{2}(E_{m} - E_{m})} \right) \\ & = \mathrm{e}^{-\beta E_{m}} \int_{0}^{\beta} \mathrm{d}\tau_{3} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} - E_{p})} \int_{\tau_{3}}^{\beta} \mathrm{d}\tau_{2} \mathrm{e}^{\tau_{2}(\omega_{2} + E_{m} - E_{m})} \int_{\tau_{2}}^{\beta} \mathrm{d}\tau_{1} \mathrm{e}^{\tau_{1}(\omega_{1} + E_{m} - E_{m})} \\ & = \mathrm{e}^{-\beta E_{m}} \int_{0}^{\beta} \mathrm{d}\tau_{3} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} - E_{p})} \int_{\tau_{3}}^{\beta} \mathrm{d}\tau_{2} \mathrm{e}^{\tau_{2}(\omega_{2} + E_{m} - E_{m})} - \mathrm{e}^{\tau_{2}(\omega_{1} + E_{m} - E_{m})} \\ & = \frac{-1}{i\omega_{1} + E_{m} - E_{n}} \int_{0}^{\beta} \mathrm{d}\tau_{3} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} - E_{p})} \int_{\tau_{3}}^{\beta} \mathrm{d}\tau_{2} \mathrm{e}^{\tau_{2}(\omega_{2} + E_{m} - E_{m})} \left( \mathrm{e}^{-\beta E_{m}} - \mathrm{e}^{\tau_{2}(\omega_{1} + E_{m} - E_{m})} - \mathrm{e}^{\tau_{2}(\omega_{1} + E_{m} - E_{m})} \right) \\ & = \frac{-1}{i\omega_{1} + E_{m} - E_{n}} \int_{0}^{\beta} \mathrm{d}\tau_{3} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} - E_{p})} \left( \mathrm{e}^{-\beta E_{m}} - \mathrm{e}^{-\beta (E_{m} - E_{m})} - \mathrm{e}^{\tau_{3}(\omega_{2} + E_{m} - E_{m})} \right) \\ & = \frac{-1}{i\omega_{1} + E_{m} - E_{n}} \int_{0}^{\beta} \mathrm{d}\tau_{3} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} - E_{p})} \left( \mathrm{e}^{-\beta E_{m}} - \mathrm{e}^{-\beta (E_{m} - E_{m})} - \mathrm{e}^{\tau_{3}(\omega_{2} + E_{m} - E_{m})} \right) \\ & = \frac{1}{i\omega_{1} + E_{m} - E_{n}} \int_{0}^{\beta} \mathrm{d}\tau_{3} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} - E_{p})} \left( \mathrm{e}^{-\beta E_{m}} - \mathrm{e}^{-\beta (E_{m} - E_{m})} - \mathrm{e}^{\tau_{3}(\omega_{2} + E_{m} - E_{m})} \right) \\ & = \frac{1}{i\omega_{1} + E_{m} - E_{n}} \left( \int_{0}^{\beta} \mathrm{d}\tau_{3} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} - E_{p})} \left[ \mathrm{e}^{-\beta E_{m}} + \mathrm{e}^{-\beta E_{m}} \mathrm{e}^{\tau_{3}(\omega_{3} + \omega_{3} + E_{m} - E_{m})} \right] \right) \\ & = \frac{1}{i\omega_{1} + E_{m} - E_{n}} \left( \int_{0}^{\beta} \mathrm{d}\tau_{3} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} - E_{p})} \left[ \mathrm{e}^{-\beta E_{m}} + \mathrm{e}^{-\beta E_{m}} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} - E_{m})} \right] \right) \\ & = \frac{1}{i\omega_{1} + i\omega_{2} + E_{m} - E_{n}} \left( \int_{0}^{\beta} \mathrm{d}\tau_{3} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} - E_{p})} \left[ \mathrm{e}^{-\beta E_{m}} - \mathrm{e}^{-\beta E_{m}} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} - E_{m})} \right] \right) \\ & = \frac{1}{i\omega_{1} + i\omega_{2} + E_{m} - E_{n}} \left( \int_{0}^{\beta} \mathrm{d}\tau_{3} \mathrm{e}^{\tau_{3}(\omega_{3} + E_{m} -$$

The **second** term evaluates to

$$-\int_{0}^{\beta} d\tau_{2} e^{i\omega_{2}\tau_{2}} \int_{0}^{\beta} d\tau_{3} e^{i\omega_{3}\tau_{3}} \int_{0}^{\beta} d\tau_{1} e^{i\omega_{1}\tau_{1}} \left( e^{-\beta E_{m}} \theta_{\tau_{1} > \tau_{3} > \tau_{2}} e^{\tau_{1}(E_{m} - E_{n})} e^{\tau_{3}(E_{n} - E_{o})} e^{\tau_{2}(E_{o} - E_{p})} \right)$$

$$= -e^{-\beta E_{m}} \int_{0}^{\beta} d\tau_{2} e^{\tau_{2}(i\omega_{2} + E_{o} - E_{p})} \int_{0}^{\beta} d\tau_{3} e^{\tau_{3}(i\omega_{3} + E_{n} - E_{o})} \int_{0}^{\beta} d\tau_{1} e^{\tau_{1}(i\omega_{1} + E_{m} - E_{n})}, \quad (1.29)$$

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  $f(\omega_1, \omega_3, \omega_2)$ , where we have defined

$$f(\omega_{1}, \omega_{2}, \omega_{3}) = \frac{1}{i\omega_{1} + E_{m} - E_{n}} \left( \frac{1}{i\omega_{2} + E_{n} - E_{o}} \left[ \frac{e^{-\beta E_{o}} + e^{-\beta E_{p}}}{i\omega_{3} + E_{o} - E_{p}} + \frac{e^{-\beta E_{n}} - e^{-\beta E_{p}}}{i\omega_{2} + i\omega_{3} + E_{n} - E_{p}} \right] - \frac{1}{i\omega_{1} + i\omega_{2} + E_{m} - E_{o}} \left[ \frac{e^{-\beta E_{o}} + e^{-\beta E_{p}}}{i\omega_{3} + E_{o} - E_{p}} - \frac{e^{-\beta E_{m}} + e^{-\beta E_{p}}}{i\omega_{1} + i\omega_{2} + i\omega_{3} + E_{m} - E_{p}} \right] \right).$$

$$(1.30)$$

For the <u>third</u> term we have to swap  $i\omega_1 \leftrightarrow i\omega_2$  compared to the first term and obtain  $f(\omega_2, \omega_1, \omega_3)$ 

For the <u>fourth</u> term we have to swap  $i\omega_1 \leftrightarrow i\omega_3$  compared to the third term and obtain  $-f(\omega_2, \omega_3, \omega_1)$ 

For the <u>fifth</u> term we have to swap  $i\omega_2 \leftrightarrow i\omega_3$  compared to the third term and obtain  $-f(\omega_3, \omega_1, \omega_2)$ 

For the <u>sixth</u> term we have to swap  $i\omega_1 \leftrightarrow i\omega_2$  compared to the fifth term and obtain  $f(\omega_3, \omega_2, \omega_1)$ 

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

$$G_{\uparrow\downarrow}^{(2)}(\omega_{1},\omega_{2},\omega_{3}) = \sum_{mnop} \left( -\langle m|c_{\uparrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}|o\rangle \langle o|c_{\downarrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{1},\omega_{2},\omega_{3}) \right)$$

$$+ \langle m|c_{\uparrow}^{\dagger}|n\rangle \langle n|c_{\downarrow}^{\dagger}|o\rangle \langle o|c_{\uparrow}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{1},\omega_{3},\omega_{2})$$

$$+ \langle m|c_{\uparrow}|n\rangle \langle n|c_{\uparrow}^{\dagger}|o\rangle \langle o|c_{\downarrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{2},\omega_{1},\omega_{3})$$

$$- \langle m|c_{\uparrow}|n\rangle \langle n|c_{\downarrow}^{\dagger}|o\rangle \langle o|c_{\uparrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{2},\omega_{3},\omega_{1})$$

$$- \langle m|c_{\downarrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}^{\dagger}|o\rangle \langle o|c_{\uparrow}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{3},\omega_{1},\omega_{2})$$

$$+ \langle m|c_{\downarrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}|o\rangle \langle o|c_{\uparrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{3},\omega_{2},\omega_{1})$$

$$+ \langle m|c_{\downarrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}|o\rangle \langle o|c_{\uparrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{3},\omega_{2},\omega_{1})$$

$$+ \langle m|c_{\downarrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}|o\rangle \langle o|c_{\uparrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{3},\omega_{2},\omega_{1})$$

$$+ \langle m|c_{\downarrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}|o\rangle \langle o|c_{\uparrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{3},\omega_{2},\omega_{1})$$

$$+ \langle m|c_{\downarrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}|o\rangle \langle o|c_{\uparrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{3},\omega_{2},\omega_{1})$$

$$+ \langle m|c_{\downarrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}|o\rangle \langle o|c_{\uparrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{3},\omega_{2},\omega_{1})$$

$$+ \langle m|c_{\downarrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}|o\rangle \langle o|c_{\uparrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{3},\omega_{2},\omega_{1})$$

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

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

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

$$(1): m(N,S) \to p(N-1,S+1) \to o(N,S) \qquad \to n(N-1,S-1) \to m(N,S)$$

$$(3): m(N,S) \to p(N-1,S+1) \to o(N,S) \qquad \to n(N+1,S+1) \to m(N,S)$$

$$(4): m(N,S) \to p(N-1,S+1) \to o(N,S+2) \qquad \to n(N+1,S+1) \to m(N,S)$$

$$(6): m(N,S) \to p(N-1,S+1) \to o(N,S+2) \qquad \to n(N-1,S+1) \to m(N,S)$$

$$(2): m(N,S) \to p(N-1,S+1) \to o(N-2,S) \qquad \to n(N-1,S-1) \to m(N,S)$$

$$(5): m(N,S) \to p(N-1,S+1) \to o(N-2,S) \qquad \to n(N-1,S+1) \to m(N,S)$$

$$(1.33)$$

which results in the final expression to be evaluated

$$G_{\uparrow\downarrow}^{(2)}(\omega_{1},\omega_{2},\omega_{3}) = \sum_{mnop} \left( -\langle m|c_{\uparrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}|o\rangle \langle o|c_{\downarrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{1},\omega_{2},\omega_{3}) \right)$$

$$+ \langle m|c_{\uparrow}|n\rangle \langle n|c_{\uparrow}^{\dagger}|o\rangle \langle o|c_{\downarrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{2},\omega_{1},\omega_{3})$$

$$- \langle m|c_{\uparrow}|n\rangle \langle n|c_{\downarrow}^{\dagger}|o\rangle \langle o|c_{\uparrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{2},\omega_{3},\omega_{1})$$

$$+ \langle m|c_{\downarrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}|o\rangle \langle o|c_{\uparrow}^{\dagger}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{3},\omega_{2},\omega_{1})$$

$$+ \langle m|c_{\uparrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}^{\dagger}|o\rangle \langle o|c_{\uparrow}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{1},\omega_{3},\omega_{2})$$

$$- \langle m|c_{\downarrow}^{\dagger}|n\rangle \langle n|c_{\uparrow}^{\dagger}|o\rangle \langle o|c_{\uparrow}|p\rangle \langle p|c_{\downarrow}|m\rangle f(\omega_{3},\omega_{1},\omega_{2}) \right). \quad (1.34)$$