

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

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

$$= -i\theta(t - t') \left(\langle c_a(t) c_b^\dagger(t') \rangle - \langle c_b^\dagger(t') c_a(t) \rangle \right) \quad (1.2)$$

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

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

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

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

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

In the same way we get for the second term

$$G_{ab}^<(t, t') = i \langle c_b^\dagger(t') c_a(t) \rangle \quad (1.7)$$

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

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

The full retarded Green's function is then given by

$$G_{ab}^R(t - t') = \theta(t - t') \frac{-i}{Z} \sum_{n,m} (e^{-\beta E_n} + e^{-\beta E_m}) e^{i(E_n - E_m)(t - t')} \langle n | c_a | m \rangle \langle m | c_b^\dagger | n \rangle. \quad (1.10)$$

A Fourier transform to frequency space yields

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

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

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

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

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

The other spin combinations like $\uparrow\uparrow$ can be 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 τ_1, τ_2, τ_3

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

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

$$\begin{aligned}
& \sum_{mnop} e^{-\beta E_m} \left(+ \theta_{\tau_1 > \tau_2 > \tau_3} \langle m | c_{\uparrow}^{\dagger}(\tau_1) | n \rangle \langle n | c_{\uparrow}(\tau_2) | o \rangle \langle o | c_{\downarrow}^{\dagger}(\tau_3) | p \rangle \langle p | c_{\downarrow}(0) | m \rangle \right. \\
& - \theta_{\tau_1 > \tau_3 > \tau_2} \langle m | c_{\uparrow}^{\dagger}(\tau_1) | n \rangle \langle n | c_{\downarrow}^{\dagger}(\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_{\uparrow}^{\dagger}(\tau_1) | o \rangle \langle o | c_{\downarrow}^{\dagger}(\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_{\downarrow}^{\dagger}(\tau_3) | o \rangle \langle o | c_{\uparrow}^{\dagger}(\tau_1) | p \rangle \langle p | c_{\downarrow}(0) | m \rangle \\
& + \theta_{\tau_3 > \tau_1 > \tau_2} \langle m | c_{\downarrow}^{\dagger}(\tau_3) | n \rangle \langle n | c_{\uparrow}^{\dagger}(\tau_1) | o \rangle \langle o | c_{\uparrow}(\tau_2) | p \rangle \langle p | c_{\downarrow}(0) | m \rangle \\
& \left. - \theta_{\tau_3 > \tau_2 > \tau_1} \langle m | c_{\downarrow}^{\dagger}(\tau_3) | n \rangle \langle n | c_{\uparrow}(\tau_2) | o \rangle \langle o | c_{\uparrow}^{\dagger}(\tau_1) | p \rangle \langle p | c_{\downarrow}(0) | m \rangle \right) \tag{1.16} \\
= & \sum_{mnop} e^{-\beta E_m} \left(+ \theta_{\tau_1 > \tau_2 > \tau_3} e^{\tau_1(E_m - E_n)} e^{\tau_2(E_n - E_o)} e^{\tau_3(E_o - E_p)} \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 \right. \\
& - \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)} \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 \\
& - \theta_{\tau_2 > \tau_1 > \tau_3} e^{\tau_2(E_m - E_n)} e^{\tau_1(E_n - E_o)} e^{\tau_3(E_o - E_p)} \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 \\
& + \theta_{\tau_2 > \tau_3 > \tau_1} e^{\tau_2(E_m - E_n)} e^{\tau_3(E_n - E_o)} e^{\tau_1(E_o - E_p)} \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 \\
& + \theta_{\tau_3 > \tau_1 > \tau_2} e^{\tau_3(E_m - E_n)} e^{\tau_1(E_n - E_o)} e^{\tau_2(E_o - E_p)} \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 \\
& \left. - \theta_{\tau_3 > \tau_2 > \tau_1} e^{\tau_3(E_m - E_n)} e^{\tau_2(E_n - E_o)} e^{\tau_1(E_o - E_p)} \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 \right). \tag{1.17}
\end{aligned}$$

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

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

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

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

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

$$= \frac{-1}{i\omega_1 + E_m - E_n} \int_0^\beta d\tau_3 e^{\tau_3(i\omega_3 + E_o - E_p)} \left(e^{-\beta E_n} \frac{-e^{\beta(E_n - E_o)} - e^{\tau_3(i\omega_2 + E_n - E_o)}}{i\omega_2 + E_n - E_o} + e^{-\beta E_m} \frac{e^{\beta(E_m - E_o)} - e^{\tau_3(i\omega_1 + i\omega_2 + E_m - E_o)}}{i\omega_1 + i\omega_2 + E_m - E_o} \right) \quad (1.22)$$

$$= \frac{1}{i\omega_1 + E_m - E_n} \int_0^\beta d\tau_3 e^{\tau_3(i\omega_3 + E_o - E_p)} \left(\frac{e^{-\beta E_o} + e^{-\beta E_n} e^{\tau_3(i\omega_2 + E_n - E_o)}}{i\omega_2 + E_n - E_o} - \frac{e^{-\beta E_o} - e^{-\beta E_m} e^{\tau_3(i\omega_1 + i\omega_2 + E_m - E_o)}}{i\omega_1 + i\omega_2 + E_m - E_o} \right) \quad (1.23)$$

$$= \frac{1}{i\omega_1 + E_m - E_n} \left(\frac{\int_0^\beta d\tau_3 e^{\tau_3(i\omega_3 + E_o - E_p)} \left[e^{-\beta E_o} + e^{-\beta E_n} e^{\tau_3(i\omega_2 + E_n - E_o)} \right]}{i\omega_2 + E_n - E_o} - \frac{\int_0^\beta d\tau_3 e^{\tau_3(i\omega_3 + E_o - E_p)} \left[e^{-\beta E_o} - e^{-\beta E_m} e^{\tau_3(i\omega_1 + i\omega_2 + E_m - E_o)} \right]}{i\omega_1 + i\omega_2 + E_m - E_o} \right) \quad (1.24)$$

$$= \frac{1}{i\omega_1 + E_m - E_n} \left(\frac{1}{i\omega_2 + E_n - E_o} \left[e^{-\beta E_o} \frac{-e^{\beta(E_o - E_p)} - 1}{i\omega_3 + E_o - E_p} + e^{-\beta E_n} \frac{e^{\beta(E_n - E_p)} - 1}{i\omega_2 + i\omega_3 + E_n - E_p} \right] - \frac{1}{i\omega_1 + i\omega_2 + E_m - E_o} \left[e^{-\beta E_o} \frac{-e^{\beta(E_o - E_p)} - 1}{i\omega_3 + E_o - E_p} - e^{-\beta E_m} \frac{-e^{\beta(E_m - E_p)} - 1}{i\omega_1 + i\omega_2 + i\omega_3 + E_m - E_p} \right] \right) \quad (1.25)$$

$$= \frac{1}{i\omega_1 + E_m - E_n} \left(\frac{1}{i\omega_2 + E_n - E_o} \left[\frac{-e^{-\beta E_p} - e^{-\beta E_o}}{i\omega_3 + E_o - E_p} + \frac{e^{-\beta E_p} - e^{-\beta E_n}}{i\omega_2 + i\omega_3 + E_n - E_p} \right] - \frac{1}{i\omega_1 + i\omega_2 + E_m - E_o} \left[\frac{-e^{-\beta E_p} - e^{-\beta E_o}}{i\omega_3 + E_o - E_p} - \frac{-e^{-\beta E_p} - e^{-\beta E_m}}{i\omega_1 + i\omega_2 + i\omega_3 + E_m - E_p} \right] \right) \quad (1.26)$$

$$= \frac{-1}{i\omega_1 + E_m - E_n} \left(\frac{1}{i\omega_2 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_3 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_2 + i\omega_3 + E_n - E_p} \right] - \frac{1}{i\omega_1 + i\omega_2 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_3 + E_o - E_p} - \frac{e^{-\beta E_m} + e^{-\beta E_p}}{i\omega_1 + i\omega_2 + i\omega_3 + E_m - E_p} \right] \right). \quad (1.27)$$

The **second** term evaluates to

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

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

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

$$\begin{aligned} & \frac{1}{i\omega_1 + E_m - E_n} \left(\frac{1}{i\omega_3 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_2 + i\omega_3 + E_n - E_p} \right] \right. \\ & \quad \left. - \frac{1}{i\omega_1 + i\omega_3 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + E_o - E_p} - \frac{e^{-\beta E_m} + e^{-\beta E_p}}{i\omega_1 + i\omega_2 + i\omega_3 + E_m - E_p} \right] \right). \end{aligned} \quad (1.30)$$

For the **third** term we have to swap $i\omega_1 \leftrightarrow i\omega_2$ compared to the first term and obtain

$$\begin{aligned} & \frac{1}{i\omega_2 + E_m - E_n} \left(\frac{1}{i\omega_1 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_3 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_1 + i\omega_3 + E_n - E_p} \right] \right. \\ & \quad \left. - \frac{1}{i\omega_1 + i\omega_2 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_3 + E_o - E_p} - \frac{e^{-\beta E_m} + e^{-\beta E_p}}{i\omega_1 + i\omega_2 + i\omega_3 + E_m - E_p} \right] \right). \end{aligned} \quad (1.31)$$

For the **fourth** term we have to swap $i\omega_1 \leftrightarrow i\omega_3$ compared to the third term and obtain

$$\begin{aligned} & \frac{-1}{i\omega_2 + E_m - E_n} \left(\frac{1}{i\omega_3 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_1 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_1 + i\omega_3 + E_n - E_p} \right] \right. \\ & \quad \left. - \frac{1}{i\omega_3 + i\omega_2 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_1 + E_o - E_p} - \frac{e^{-\beta E_m} + e^{-\beta E_p}}{i\omega_1 + i\omega_2 + i\omega_3 + E_m - E_p} \right] \right). \end{aligned} \quad (1.32)$$

For the **fifth** term we have to swap $i\omega_2 \leftrightarrow i\omega_3$ compared to the third term and obtain

$$\begin{aligned} & \frac{-1}{i\omega_3 + E_m - E_n} \left(\frac{1}{i\omega_1 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_1 + i\omega_2 + E_n - E_p} \right] \right. \\ & \quad \left. - \frac{1}{i\omega_1 + i\omega_3 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + E_o - E_p} - \frac{e^{-\beta E_m} + e^{-\beta E_p}}{i\omega_1 + i\omega_2 + i\omega_3 + E_m - E_p} \right] \right). \end{aligned} \quad (1.33)$$

For the **sixth** term we have to swap $i\omega_1 \leftrightarrow i\omega_2$ compared to the fifth term and obtain

$$\begin{aligned} & \frac{1}{i\omega_3 + E_m - E_n} \left(\frac{1}{i\omega_2 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_1 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_1 + i\omega_2 + E_n - E_p} \right] \right. \\ & \quad \left. - \frac{1}{i\omega_2 + i\omega_3 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_1 + E_o - E_p} - \frac{e^{-\beta E_m} + e^{-\beta E_p}}{i\omega_1 + i\omega_2 + i\omega_3 + E_m - E_p} \right] \right). \end{aligned} \quad (1.34)$$

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

$$\begin{aligned}
G_{\uparrow\downarrow}^{(2)}(\omega_1, \omega_2, \omega_3) = \sum_{mnop} \Bigg(& \\
& - \frac{\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}{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] \right. \\
& \quad \left. - \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) \\
& + \frac{\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}{i\omega_1 + E_m - E_n} \left(\frac{1}{i\omega_3 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_2 + i\omega_3 + E_n - E_p} \right] \right. \\
& \quad \left. - \frac{1}{i\omega_1 + i\omega_3 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + 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) (2) \\
& + \frac{\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}{i\omega_2 + E_m - E_n} \left(\frac{1}{i\omega_1 + 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_1 + i\omega_3 + E_n - E_p} \right] \right. \\
& \quad \left. - \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) (3) \\
& - \frac{\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}{i\omega_2 + E_m - E_n} \left(\frac{1}{i\omega_3 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_1 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_1 + i\omega_3 + E_n - E_p} \right] \right. \\
& \quad \left. - \frac{1}{i\omega_3 + i\omega_2 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_1 + 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) (4) \\
& - \frac{\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}{i\omega_3 + E_m - E_n} \left(\frac{1}{i\omega_1 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_1 + i\omega_2 + E_n - E_p} \right] \right. \\
& \quad \left. - \frac{1}{i\omega_1 + i\omega_3 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + 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) (5) \\
& + \frac{\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}{i\omega_3 + 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_1 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_1 + i\omega_2 + E_n - E_p} \right] \right. \\
& \quad \left. - \frac{1}{i\omega_2 + i\omega_3 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_1 + 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) (6) \Bigg).
\end{aligned}$$

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

$$\begin{aligned}
(1) : & m(N, S) \rightarrow p(N-1, S+1) \rightarrow o(N, S) \rightarrow n(N-1, S-1) \rightarrow m(N, S) \\
(2) : & m(N, S) \rightarrow p(N-1, S+1) \rightarrow o(N-2, S) \rightarrow n(N-1, S-1) \rightarrow m(N, S) \\
(3) : & m(N, S) \rightarrow p(N-1, S+1) \rightarrow o(N, S) \rightarrow n(N+1, S+1) \rightarrow m(N, S) \\
(4) : & m(N, S) \rightarrow p(N-1, S+1) \rightarrow o(N, S+2) \rightarrow n(N+1, S+1) \rightarrow m(N, S) \\
(5) : & m(N, S) \rightarrow p(N-1, S+1) \rightarrow o(N-2, S) \rightarrow n(N-1, S+1) \rightarrow m(N, S) \\
(6) : & m(N, S) \rightarrow p(N-1, S+1) \rightarrow o(N, S+2) \rightarrow n(N-1, S+1) \rightarrow m(N, S)
\end{aligned} \tag{1.35}$$

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

$$\begin{aligned}
(1) : m(N, S) &\rightarrow p(N-1, S+1) \rightarrow o(N, S) && \rightarrow n(N-1, S-1) \rightarrow m(N, S) \\
(3) : m(N, S) &\rightarrow p(N-1, S+1) \rightarrow o(N, S) && \rightarrow n(N+1, S+1) \rightarrow m(N, S) \\
(4) : m(N, S) &\rightarrow p(N-1, S+1) \rightarrow o(N, S+2) && \rightarrow n(N+1, S+1) \rightarrow m(N, S) \\
(6) : m(N, S) &\rightarrow p(N-1, S+1) \rightarrow o(N, S+2) && \rightarrow n(N-1, S+1) \rightarrow m(N, S) \\
(2) : m(N, S) &\rightarrow p(N-1, S+1) \rightarrow o(N-2, S) && \rightarrow n(N-1, S-1) \rightarrow m(N, S) \\
(5) : m(N, S) &\rightarrow p(N-1, S+1) \rightarrow o(N-2, S) && \rightarrow n(N-1, S+1) \rightarrow m(N, S)
\end{aligned} \tag{1.36}$$

which results in the final expression to be evaluated

$$\begin{aligned}
G_{\uparrow\downarrow}^{(2)}(\omega_1, \omega_2, \omega_3) = \frac{1}{Z} \sum_{mnop} \bigg(& \\
& - \frac{\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}{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] \right. \\
& \quad \left. - \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) \\
& + \frac{\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}{i\omega_2 + E_m - E_n} \left(\frac{1}{i\omega_1 + 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_1 + i\omega_3 + E_n - E_p} \right] \right. \\
& \quad \left. - \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) (3) \\
& - \frac{\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}{i\omega_2 + E_m - E_n} \left(\frac{1}{i\omega_3 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_1 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_1 + i\omega_3 + E_n - E_p} \right] \right. \\
& \quad \left. - \frac{1}{i\omega_3 + i\omega_2 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_1 + 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) (4) \\
& + \frac{\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}{i\omega_3 + 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_1 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_1 + i\omega_2 + E_n - E_p} \right] \right. \\
& \quad \left. - \frac{1}{i\omega_2 + i\omega_3 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_1 + 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) (6) \\
& + \frac{\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}{i\omega_1 + E_m - E_n} \left(\frac{1}{i\omega_3 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_2 + i\omega_3 + E_n - E_p} \right] \right. \\
& \quad \left. - \frac{1}{i\omega_1 + i\omega_3 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + 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) (2) \\
& - \frac{\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}{i\omega_3 + E_m - E_n} \left(\frac{1}{i\omega_1 + E_n - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + E_o - E_p} + \frac{e^{-\beta E_n} - e^{-\beta E_p}}{i\omega_1 + i\omega_2 + E_n - E_p} \right] \right. \\
& \quad \left. - \frac{1}{i\omega_1 + i\omega_3 + E_m - E_o} \left[\frac{e^{-\beta E_o} + e^{-\beta E_p}}{i\omega_2 + 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) (5) \bigg).
\end{aligned}$$