

Supplement Material for Manuscript

“Ultrafast Dynamics of Strongly Correlated Fermions — Nonequilibrium Green Functions and Selfenergy Approximations”

N. Schluenzen, S. Hermanns, M. Scharnke, and M. Bonitz

Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

1. Derivations in full notation

For the following derivations we repeat several equations from the main text. From Hedin’s equations (or the respective scheme for the bare interaction) we rewrite the Dyson equation [main text: Eq. (91)],

$$G_{ij}(z_1, z_2) = G_{ij}^{(0)}(z_1, z_2) + \int_{\mathcal{C}} dz_3 dz_4 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \Sigma_{mn}(z_3, z_4) G_{nj}(z_4, z_2), \quad (1)$$

the selfenergy [main text: Eqs. (95), (97) and (101)],

$$\Sigma_{ij}(z_1, z_2) = \Sigma_{ij}^H(z_1, z_2) + \Sigma_{ij}^{xc}(z_1, z_2), \quad (2)$$

$$\Sigma_{ij}^{xc}(z_1, z_2) = i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \Lambda_{nqpj}(z_3, z_2, z_1), \quad (3)$$

$$\begin{aligned} \Sigma_{ij}^{xc}(z_1, z_2) &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}(z_1, z_3) \times \\ &\quad \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}(z_4, z_2, z_3), \end{aligned} \quad (4)$$

the interaction [main text: Eqs. (102)-(104)],

$$W_{ijkl}(z_1, z_2) = W_{ijkl}^{\text{bare}}(z_1, z_2) + W_{ijkl}^{\text{ns}}(z_1, z_2), \quad (5)$$

$$W_{ijkl}^{(1)}(z_1, z_2) = W_{ijkl}^{\text{bare}}(z_1, z_2) = \delta_{\mathcal{C}}(z_1, z_2) w_{ijkl}(z_1), \quad (6)$$

$$W_{ijkl}^{\text{ns}}(z_1, z_2) = \sum_{mn} w_{imnl}(z_1) \int_C dz_3 \sum_{pq} P_{nqpm}(z_1, z_3) W_{pjkl}(z_3, z_2), \quad (7)$$

and the polarizability [main text: Eq. (105)],

$$\begin{aligned} P_{ijkl}(z_1, z_2) &= \pm i\hbar \int_C dz_3 \sum_m G_{im}(z_1, z_3) \times \\ &\quad \int_C dz_4 \sum_n G_{nl}(z_4, z_1) \Gamma_{mjkn}(z_3, z_4, z_2). \end{aligned} \quad (8)$$

The first-order selfenergy reads [main text: Eq. (158)]

$$\Sigma_{ij}^{(1)}(z_1, z_2) = \Sigma_{ij}^H(z_1, z_2) + \Sigma_{ij}^F(z_1, z_2), \quad (9)$$

with [main text: Eq. (156)]

$$\begin{aligned} \Sigma_{ij}^F(z_1, z_2) &= \Sigma_{ij}^{\text{xc}}(W^{(1)} \equiv W^{\text{bare}}, \Gamma^{(0)}) = \\ &= i\hbar \delta_C(z_1, z_2) \sum_{mn} w_{injm}(z_1) G_{mn}(z_1, z_{1+}). \end{aligned} \quad (10)$$

The zeroth-order screened vertex becomes [main text: Eq. (155)]

$$\Gamma_{ijkl}^{(0)}(z_1, z_2, z_3) = \delta_C(z_1, z_{2+}) \delta_C(z_3, z_2) \delta_{ik} \delta_{jl}. \quad (11)$$

1.1. Second-order selfenergy contributions

1.1.1. Direct second-order selfenergy

The first second-order selfenergy term involves $W^{(2)}$, which structurally is given by, cf. Eq. (5),

$$W^{(2)} = W^{\text{ns}}(P^{(0)}, W^{(1)}). \quad (12)$$

The structure of the zeroth-order term of the polarization is

$$P^{(0)} = P(\Gamma^{(0)}). \quad (13)$$

Thus, it is given by

$$\begin{aligned} P_{ijkl}^{(0)}(z_1, z_2) &= \pm i\hbar \int_C dz_3 \sum_m G_{im}(z_1, z_3) \\ &\quad \int_C dz_4 \sum_n G_{nl}(z_4, z_1) \delta_C(z_3, z_{4+}) \delta_C(z_2, z_4) \delta_{mk} \delta_{jn} \\ &= \pm i\hbar G_{ik}(z_1, z_2) G_{jl}(z_2, z_1). \end{aligned} \quad (14)$$

Inserting this result into Eq. (12), one arrives at

$$\begin{aligned} W_{ijkl}^{(2)}(z_1, z_2) &= \sum_{mn} w_{imnl}(z_1) \\ &\quad \int_C dz_3 \sum_{pq} (\pm i\hbar G_{np}(z_1, z_3) G_{qm}(z_3, z_1)) \delta_C(z_3, z_2) w_{pjkl}(z_3) \end{aligned} \quad (15)$$

and, employing Eq. (7), finally, one has

$$\begin{aligned} W_{ijkl}^{(2)}(z_1, z_2) &= \pm i\hbar \sum_{mn} w_{imnl}(z_1) \sum_{pq} G_{np}(z_1, z_2) G_{qm}(z_2, z_1) w_{pjkl}(z_2). \end{aligned} \quad (16)$$

With this, $\Sigma^{(2),2,0}$ can be calculated as, cf. Eq. (4),

$$\begin{aligned} \Sigma_{ij}^{(2),2,0}(z_1, z_2) &= \pm i\hbar \int_C dz_3 \sum_{mpq} \left(\pm i\hbar \sum_{rs} w_{irs}(z_1) \sum_{tu} G_{st}(z_1, z_3) G_{ur}(z_3, z_1) w_{tpqu}(z_3) \right) \\ &\quad \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \delta_C(z_4, z_2+) \delta_C(z_3, z_2) \delta_{np} \delta_{qj}. \end{aligned} \quad (17)$$

Evaluating the terms, one arrives at

$$\begin{aligned} \Sigma_{ij}^{(2),2,0}(z_1, z_2) &= \pm (i\hbar)^2 \sum_{mn} G_{mn}(z_1, z_2) \sum_{st} G_{st}(z_1, z_2) \\ &\quad \sum_r w_{irs}(z_1) \sum_u w_{tnju}(z_2) G_{ur}(z_2, z_1). \end{aligned} \quad (18)$$

1.1.2. Exchange-correlation second-order selfenergy

The other second-order selfenergy term, $\Sigma_{ij}^{(2),1,1}$, requires the first-order term of the vertex Γ , the structure of which is

$$\Gamma^{(1)} = \Gamma(\delta\Sigma^{\text{xc},(1)}/\delta G, \Gamma^{(0)}). \quad (19)$$

This term involves the functional derivative of $\Sigma^{\text{xc},(1)}$ with respect to G . One has

$$\frac{\delta\Sigma_{ij}^{\text{xc},(1)}(z_1, z_2)}{\delta G_{rs}(z_5, z_6)} = \frac{\delta\Sigma_{ij}^{\text{xc},(1),F}(z_1, z_2)}{\delta G_{rs}(z_5, z_6)}. \quad (20)$$

Employing Eq. (10), one finds

$$\begin{aligned} \frac{\delta\Sigma_{ij}^{\text{xc},(1)}(z_1, z_2)}{\delta G_{rs}(z_5, z_6)} &= i\hbar \delta_C(z_1, z_2) \sum_{mn} w_{injm}(z_1) \frac{\delta G_{mn}(z_1, z_1+)}{\delta G_{rs}(z_5, z_6)} \\ &= i\hbar \delta_C(z_1, z_2) \delta_C(z_1, z_5) \delta_C(z_1, z_6) w_{isjr}(z_1), \end{aligned} \quad (21)$$

where

$$\frac{\delta G_{ij}(z_1, z_2)}{\delta G_{mn}(z_5, z_6)} = \delta_C(z_1, z_5) \delta_C(z_2, z_6) \delta_{im} \delta_{jn} \quad (22)$$

has been applied. With this,

$$\begin{aligned} & \Gamma_{ijkl}^{(1)}(z_1, z_2, z_3) \\ &= \int_C dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}^{\text{xc},(1)}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_C dz_6 \sum_p G_{mp}(z_4, z_6) \\ & \quad \int_C dz_7 \sum_q G_{qn}(z_7, z_5) \Gamma_{pjkl}^{(0)}(z_6, z_7, z_3). \end{aligned} \quad (23)$$

Using Eq. (21), one has

$$\begin{aligned} & \Gamma_{ijkl}^{(1)}(z_1, z_2, z_3) \\ &= i\hbar \delta_C(z_1, z_2) \sum_{mn} w_{inlm}(z_1) \int_C dz_6 \sum_p G_{mp}(z_1, z_6) \\ & \quad \int_C dz_7 \sum_q G_{qn}(z_7, z_1) \Gamma_{pjkl}^{(0)}(z_6, z_7, z_3). \end{aligned} \quad (24)$$

With Eq. (11), finally,

$$\begin{aligned} & \Gamma_{ijkl}^{(1)}(z_1, z_2, z_3) \\ &= i\hbar \delta_C(z_1, z_2) \sum_{mn} w_{inlm}(z_1) G_{mk}(z_1, z_3) G_{jn}(z_3, z_1) \end{aligned} \quad (25)$$

ensues. Inserting this result yields

$$\begin{aligned} & \Sigma_{ij}^{(2),1,1}(z_1, z_2) \\ &= i\hbar \int_C dz_3 \sum_{mpq} W_{ipqm}^{(1)}(z_1, z_3) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(1)}(z_4, z_2, z_3). \end{aligned} \quad (26)$$

Employing Eqs. (6) and (25), one arrives at

$$\begin{aligned} & \Sigma_{ij}^{(2),1,1}(z_1, z_2) \\ &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(1)}(z_4, z_2, z_1) \\ &= (i\hbar)^2 \sum_{mpq} w_{ipqm}(z_1) \sum_n G_{mn}(z_1, z_2) \sum_{rs} w_{nsjr}(z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_2). \end{aligned} \quad (27)$$

1.2. Third-order selfenergy contributions

1.2.1. Third-order term: $\Sigma_{ij}^{(3),\{3;0,2\},0}$

Using Eq. (7), one finds

$$\begin{aligned} W_{ijkl}^{(3),0,2}(z_1, z_2) \\ = \sum_{mn} w_{imnl}(z_1) \int_C dz_3 \sum_{pq} (\pm i\hbar G_{np}(z_1, z_3) G_{qm}(z_3, z_1)) W_{pjkl}^{(2)}(z_3, z_2). \end{aligned} \quad (28)$$

Employing Eq. (15) yields

$$\begin{aligned} W_{ijkl}^{(3),0,2}(z_1, z_2) \\ = \sum_{mn} w_{imnl}(z_1) \int_C dz_3 \sum_{pq} (\pm i\hbar G_{np}(z_1, z_3) G_{qm}(z_3, z_1)) \\ \left(\pm i\hbar \sum_{rs} w_{prs}(z_3) \sum_{tu} G_{st}(z_3, z_2) G_{ur}(z_2, z_3) w_{tjku}(z_2) \right). \end{aligned} \quad (29)$$

Evaluating and reordering, one has

$$\begin{aligned} W_{ijkl}^{(3),0,2}(z_1, z_2) \\ = (i\hbar)^2 \sum_{mn} w_{imnl}(z_1) \int_C dz_3 \sum_{pq} G_{np}(z_1, z_3) G_{qm}(z_3, z_1) \sum_{rs} w_{prs}(z_3) \\ \sum_{tu} G_{st}(z_3, z_2) G_{ur}(z_2, z_3) w_{tjku}(z_2). \end{aligned} \quad (30)$$

With this, the first term of the first third-order selfenergy class, $\Sigma^{(3),3,0}$, becomes

$$\begin{aligned} \Sigma_{ij}^{(3),\{3;0,2\},0}(z_1, z_2) \\ = i\hbar \int_C dz_3 \sum_{mpq} W_{ipqm}^{(3),0,2}(z_1, z_3) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpl}^{(0)}(z_4, z_2, z_3). \end{aligned} \quad (31)$$

Using Eq. (11), one has

$$\begin{aligned} \Sigma_{ij}^{(3),\{3;0,2\},0}(z_1, z_2) \\ = (i\hbar)^3 \sum_{mn} G_{mn}(z_1, z_2) \sum_{rs} w_{irs}(z_1) \int_C dz_3 \sum_{tu} G_{st}(z_1, z_3) G_{ur}(z_3, z_1) \\ \sum_{vw} w_{tvwu}(z_3) \sum_{xy} G_{wx}(z_3, z_2) G_{yv}(z_2, z_3) w_{xnjy}(z_2). \end{aligned} \quad (32)$$

1.2.2. Third-order term: $\Sigma_{ij}^{(3),\{3;1,1\},0}$

For the second class of the interaction, $W^{(3),1,1}$, the first-order contribution to the polarizability is needed, which is given by, cf. Eqs. (8) and (25),

$$\begin{aligned} P_{ijkl}^{(1)}(z_1, z_2) &= P_{ijkl}(z_1, z_2)(\Gamma^{(1)}) \\ &= \pm i\hbar \int_C dz_3 \sum_m G_{im}(z_1, z_3) \int_C dz_4 \sum_n G_{nl}(z_4, z_1) \Gamma_{mjkn}^{(1)}(z_3, z_4, z_2). \end{aligned} \quad (33)$$

Employing Eq. (25), one arrives at

$$\begin{aligned} & P_{ijkl}^{(1)}(z_1, z_2) \\ &= \pm (\mathrm{i}\hbar)^2 \int_C dz_3 \sum_m G_{im}(z_1, z_3) \sum_n G_{nl}(z_3, z_1) \\ & \quad \sum_{pq} w_{mqnp}(z_3) G_{pk}(z_3, z_2) G_{jq}(z_2, z_3). \end{aligned} \tag{34}$$

Inserting this result back, one finds, using Eq. (7),

$$\begin{aligned} W_{ijkl}^{(3),1,1}(z_1, z_2) &= \sum_{mn} w_{imnl}(z_1) \int_C dz_3 \sum_{pq} P_{nqpm}^{(1)}(z_1, z_3) W_{pjkl}^{(1)}(z_3, z_2) \\ &= \sum_{mn} w_{imnl}(z_1) \int_C dz_3 \sum_{pq} \left(\pm (\mathrm{i}\hbar)^2 \int_C dz_4 \sum_r G_{nr}(z_1, z_4) \sum_s G_{sm}(z_4, z_1) \right. \\ & \quad \left. \sum_{tu} w_{rust}(z_4) G_{tp}(z_4, z_3) G_{qu}(z_3, z_4) \right) \delta_C(z_3, z_2) w_{pjkl}(z_2). \end{aligned} \tag{35}$$

After reordering, one has

$$\begin{aligned} & W_{ijkl}^{(3),1,1}(z_1, z_2) \\ &= \pm (\mathrm{i}\hbar)^2 \sum_{mn} w_{imnl}(z_1) \int_C dz_3 \sum_r G_{nr}(z_1, z_3) \sum_s G_{sm}(z_3, z_1) \\ & \quad \sum_{tu} w_{rust}(z_3) \sum_{pq} G_{tp}(z_3, z_2) G_{qu}(z_2, z_3) w_{pjkl}(z_2). \end{aligned} \tag{36}$$

With these results, the second term of the class $\Sigma^{(3),3,0}$ is found, using Eq. (4),

$$\begin{aligned} & \Sigma_{ij}^{(3),\{3;1,1\},0}(z_1, z_2) \\ &= \mathrm{i}\hbar \int_C dz_3 \sum_{mpq} W_{ipqm}^{(3),1,1}(z_1, z_3) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(0)}(z_4, z_2, z_3). \end{aligned} \tag{37}$$

Using Eq. (11), one finds

$$\begin{aligned} & \Sigma_{ij}^{(3),\{3;1,1\},0}(z_1, z_2) \\ &= \pm (\mathrm{i}\hbar)^3 \sum_{mn} G_{mn}(z_1, z_2) \sum_{rs} w_{irs}(z_1) \int_C dz_3 \sum_t G_{st}(z_1, z_3) \sum_u G_{ur}(z_3, z_1) \\ & \quad \sum_{vw} w_{twuv}(z_3) \sum_{xy} G_{vx}(z_3, z_2) G_{yw}(z_2, z_3) w_{xny}(z_2). \end{aligned} \tag{38}$$

1.2.3. Third-order term: $\Sigma_{ij}^{(3),2,1}$

Continuing with the second class $\Sigma^{(3),2,1}$, it is directly worked out by combining Eqs. (15)

and (25),

$$\begin{aligned}\Sigma_{ij}^{(3),2,1}(z_1, z_2) &= i\hbar \int_C dz_3 \sum_{mpq} W_{ipqm}^{(2)}(z_1, z_3) \\ &\quad \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(1)}(z_4, z_2, z_3).\end{aligned}\tag{39}$$

Inserting Eq. (25) yields

$$\begin{aligned}\Sigma_{ij}^{(3),2,1}(z_1, z_2) &= \pm (i\hbar)^3 \int_C dz_3 \sum_{mrs} w_{irs m}(z_1) \sum_{tu} G_{st}(z_1, z_3) G_{ur}(z_3, z_1) \sum_{pq} w_{tpqu}(z_3) \\ &\quad \sum_n G_{mn}(z_1, z_2) \sum_{vw} w_{nwjv}(z_2) G_{vp}(z_2, z_3) G_{qw}(z_3, z_2).\end{aligned}\tag{40}$$

1.2.4. Third-order term: $\Sigma_{ij}^{(3),1,\{2;1,1\}}$

For the single contribution to the class $\Gamma^{(2),1,1}$, one finds, employing Eqs. (21) and (25),

$$\begin{aligned}\Gamma_{ijkl}^{(2),1,1}(z_1, z_2, z_3) &= \int_C dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}^{\text{xc},(1)}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_C dz_6 \sum_p G_{mp}(z_4, z_6) \\ &\quad \int_C dz_7 \sum_q G_{qn}(z_7, z_5) \Gamma_{pjkq}^{(1)}(z_6, z_7, z_3).\end{aligned}\tag{41}$$

Evaluating the derivative yields

$$\begin{aligned}\Gamma_{ijkl}^{(2),1,1}(z_1, z_2, z_3) &= i\hbar \delta_C(z_1, z_2) \sum_{mn} w_{inlm}(z_1) \int_C dz_6 \sum_p G_{mp}(z_1, z_6) \\ &\quad \int_C dz_7 \sum_q G_{qn}(z_7, z_1) \Gamma_{pjkq}^{(1)}(z_6, z_7, z_3).\end{aligned}\tag{42}$$

Employing Eq. (25), one finds

$$\begin{aligned}\Gamma_{ijkl}^{(2),1,1}(z_1, z_2, z_3) &= (i\hbar)^2 \delta_C(z_1, z_2) \sum_{mn} w_{inlm}(z_1) \int_C dz_6 \sum_p G_{mp}(z_1, z_6) \\ &\quad \sum_q G_{qn}(z_6, z_1) \sum_{rs} w_{psqr}(z_6) G_{rk}(z_6, z_3) G_{js}(z_3, z_6).\end{aligned}\tag{43}$$

This enables the computation of $\Sigma^{(3),1,\{2;1,1\}}$ with Eqs. (4) and (6),

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;1,1\}}(z_1, z_2) &= i\hbar \int_C dz_3 \sum_{mpq} W_{ipqm}^{(1)}(z_1, z_3) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),1,1}(z_4, z_2, z_3) \\ &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),1,1}(z_4, z_2, z_1). \end{aligned} \quad (44)$$

Using Eq. (43), one arrives at

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;1,1\}}(z_1, z_2) &= (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \sum_n G_{mn}(z_1, z_2) \sum_{rs} w_{nsjr}(z_2) \int_C dz_3 \sum_t G_{rt}(z_2, z_3) \\ &\quad \sum_u G_{us}(z_3, z_2) \sum_{vw} w_{twuv}(z_3) G_{vp}(z_3, z_1) G_{qw}(z_1, z_3). \end{aligned} \quad (45)$$

1.2.5. Second-order vertex terms

For the first terms, one finds

$$\begin{aligned} \Gamma_{ijkl}^{(2),\{2;2,0\},0}(z_1, z_2, z_3) &= \int_C dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}^{(2),2,0}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_C dz_6 \sum_p G_{mp}(z_4, z_6) \\ &\quad \int_C dz_7 \sum_q G_{qn}(z_7, z_5) \Gamma_{pjkl}^{(0)}(z_6, z_7, z_3) \\ &= \int_C dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}^{(2),2,0}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} G_{mk}(z_4, z_3) G_{jn}(z_3, z_5). \end{aligned} \quad (46)$$

Inserting Eq. (18), the term attains the form

$$\begin{aligned} \Gamma_{ijkl}^{(2),\{2;2,0\},0}(z_1, z_2, z_3) &= \pm (i\hbar)^2 \int_C dz_4 dz_5 \\ &\quad \sum_{mn} \frac{\delta \left(\sum_{pq} G_{pq}(z_1, z_2) \sum_{st} G_{st}(z_1, z_2) \sum_r w_{irsp}(z_1) \sum_u w_{tqlu}(z_2) G_{ur}(z_2, z_1) \right)}{\delta G_{mn}(z_4, z_5)} \\ &\quad G_{mk}(z_4, z_3) G_{jn}(z_3, z_5). \end{aligned} \quad (47)$$

Evaluating the derivative, one has

$$\begin{aligned} \Gamma_{ijkl}^{(2),\{2;2,0\},0}(z_1, z_2, z_3) &= \Gamma_{ijkl}^{(2),\{2;2,0\},0,A}(z_1, z_2, z_3) \\ &\quad + \Gamma_{ijkl}^{(2),\{2;2,0\},0,B}(z_1, z_2, z_3) + \Gamma_{ijkl}^{(2),\{2;2,0\},0,C}(z_1, z_2, z_3), \end{aligned} \quad (48)$$

with

$$\begin{aligned} & \Gamma_{ijkl}^{(2),\{2;2,0\},0,A}(z_1, z_2, z_3) \\ &= \pm (i\hbar)^2 \sum_{mn} \sum_{st} G_{st}(z_1, z_2) \sum_r w_{irs m}(z_1) \\ & \quad \sum_u w_{tnlu}(z_2) G_{ur}(z_2, z_1) G_{mk}(z_1, z_3) G_{jn}(z_3, z_2) \end{aligned} \quad (49)$$

and

$$\begin{aligned} & \Gamma_{ijkl}^{(2),\{2;2,0\},0,B}(z_1, z_2, z_3) \\ &= \pm (i\hbar)^2 \sum_{mn} \sum_{pq} G_{pq}(z_1, z_2) \sum_r w_{irmp}(z_1) \\ & \quad \sum_u w_{nqlu}(z_2) G_{ur}(z_2, z_1) G_{mk}(z_1, z_3) G_{jn}(z_3, z_2) \end{aligned} \quad (50)$$

as well as

$$\begin{aligned} & \Gamma_{ijkl}^{(2),\{2;2,0\},0,C}(z_1, z_2, z_3) \\ &= \pm (i\hbar)^2 \sum_{mn} \sum_{pq} G_{pq}(z_1, z_2) \sum_{st} G_{st}(z_1, z_2) \\ & \quad w_{ins p}(z_1) w_{tqlm}(z_2) G_{mk}(z_2, z_3) G_{jn}(z_3, z_1). \end{aligned} \quad (51)$$

Similarly, one finds

$$\begin{aligned} \Gamma_{ijkl}^{(2),\{2;1,1\},0}(z_1, z_2, z_3) &= \int_C dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}^{(2),1,1}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_C dz_6 \sum_p G_{mp}(z_4, z_6) \\ & \quad \int_C dz_7 \sum_q G_{qn}(z_7, z_5) \Gamma_{pj kq}^{(0)}(z_6, z_7, z_3). \end{aligned} \quad (52)$$

Inserting Eq. (27) yields

$$\begin{aligned} \Gamma_{ijkl}^{(2),\{2;1,1\},0}(z_1, z_2, z_3) &= (i\hbar)^2 \int_C dz_4 dz_5 \\ & \quad \sum_{mn} \frac{\delta \left(\sum_{prs} w_{irs p}(z_1) \sum_q G_{pq}(z_1, z_2) \sum_{tu} w_{qult}(z_2) G_{tr}(z_2, z_1) G_{su}(z_1, z_2) \right)}{\delta G_{mn}(z_4, z_5)} \\ & \quad G_{mk}(z_4, z_3) G_{jn}(z_3, z_5), \end{aligned} \quad (53)$$

which, after evaluation of the derivative, yields

$$\begin{aligned} \Gamma_{ijkl}^{(2),\{2;1,1\},0}(z_1, z_2, z_3) &= \Gamma_{ijkl}^{(2),\{2;1,1\},0,A}(z_1, z_2, z_3) \\ &+ \Gamma_{ijkl}^{(2),\{2;1,1\},0,B}(z_1, z_2, z_3) + \Gamma_{ijkl}^{(2),\{2;1,1\},0,C}(z_1, z_2, z_3), \end{aligned} \quad (54)$$

with

$$\begin{aligned} & \Gamma_{ijkl}^{(2),\{2;1,1\},0,A}(z_1, z_2, z_3) \\ &= (\mathrm{i}\hbar)^2 \sum_{mn} \sum_{rs} w_{irs m}(z_1) \sum_{tu} w_{nult}(z_2) G_{tr}(z_2, z_1) \\ & \quad G_{su}(z_1, z_2) G_{mk}(z_1, z_3) G_{jn}(z_3, z_2) \end{aligned} \quad (55)$$

and

$$\begin{aligned} & \Gamma_{ijkl}^{(2),\{2;1,1\},0,B}(z_1, z_2, z_3) \\ &+ (\mathrm{i}\hbar)^2 \sum_{mn} \sum_{ps} w_{ins p}(z_1) \sum_q G_{pq}(z_1, z_2) \sum_u w_{qul m}(z_2) \\ & \quad G_{su}(z_1, z_2) G_{mk}(z_2, z_3) G_{jn}(z_3, z_1) \end{aligned} \quad (56)$$

as well as

$$\begin{aligned} & \Gamma_{ijkl}^{(2),\{2;1,1\},0,C}(z_1, z_2, z_3) \\ &+ (\mathrm{i}\hbar)^2 \sum_{mn} \sum_{pr} w_{irmp}(z_1) \sum_q G_{pq}(z_1, z_2) \sum_t w_{qnlt}(z_2) \\ & \quad G_{tr}(z_2, z_1) G_{mk}(z_1, z_3) G_{jn}(z_3, z_2). \end{aligned} \quad (57)$$

1.2.6. Third-order terms: $\Sigma_{ij}^{(3),1,2}$

With this result, the corresponding selfenergy terms can be computed,

$$\begin{aligned} & \Sigma_{ij}^{(3),1,\{2;\{2;2,0\},0,A\}}(z_1, z_2) \\ &= \mathrm{i}\hbar \int_C dz_3 \sum_{mpq} W_{ipqm}^{(1)}(z_1, z_3) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),\{2;2,0\},0,A}(z_4, z_2, z_3) \\ &= \mathrm{i}\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),\{2;2,0\},0,A}(z_4, z_2, z_1). \end{aligned} \quad (58)$$

Inserting Eq. (49), one arrives at

$$\begin{aligned} & \Sigma_{ij}^{(3),1,\{2;\{2;2,0\},0,A\}}(z_1, z_2) = \pm (\mathrm{i}\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \\ & \quad \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rsuv} G_{uv}(z_4, z_2) \sum_t w_{ntur}(z_4) \\ & \quad \sum_w w_{vsjw}(z_2) G_{wt}(z_2, z_4) G_{rp}(z_4, z_1) G_{qs}(z_1, z_2). \end{aligned} \quad (59)$$

For the second term, one has

$$\begin{aligned} & \Sigma_{ij}^{(3),1,\{2;\{2;2,0\},0,B\}}(z_1, z_2) \\ &= \mathrm{i}\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),\{2;2,0\},0,B}(z_4, z_2, z_1). \end{aligned} \quad (60)$$

Using Eq. (50) yields

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;\{2;2,0\},0,B\}}(z_1, z_2) \\ = \pm (\mathrm{i}\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rs} \sum_{tu} G_{tu}(z_4, z_2) \\ \sum_v w_{nvrt}(z_4) \sum_w w_{sujw}(z_2) G_{wv}(z_2, z_4) G_{rp}(z_4, z_1) G_{qs}(z_1, z_2). \end{aligned} \quad (61)$$

The third term is given by

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;\{2;2,0\},0,C\}}(z_1, z_2) \\ = \mathrm{i}\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),\{2;2,0\},0,C}(z_4, z_2, z_1). \end{aligned} \quad (62)$$

With Eq. (51), one finds

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;\{2;2,0\},0,C\}}(z_1, z_2) \\ = \pm (\mathrm{i}\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rs} \sum_{tu} G_{tu}(z_4, z_2) \\ \sum_{vw} G_{vw}(z_4, z_2) w_{nsvt}(z_4) w_{wu jr}(z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_4). \end{aligned} \quad (63)$$

For the other class, one has

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;\{2;1,1\},0,A\}}(z_1, z_2) \\ = \mathrm{i}\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}^{(1)}(z_1, z_3) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),\{2;1,1\},0,A}(z_4, z_2, z_3) \\ = \mathrm{i}\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),1,1,A}(z_4, z_2, z_1). \end{aligned} \quad (64)$$

Inserting Eq. (55) yields

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;\{2;1,1\},0,A\}}(z_1, z_2) \\ = (\mathrm{i}\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rs} \sum_{tu} w_{ntur}(z_4) \\ \sum_{vw} w_{swjv}(z_2) G_{vt}(z_2, z_4) G_{uw}(z_4, z_2) G_{rp}(z_4, z_1) G_{qs}(z_1, z_2). \end{aligned} \quad (65)$$

Similarly, the second term reads

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;\{2;1,1\},0,B\}}(z_1, z_2) \\ = \mathrm{i}\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),\{2;1,1\},0,B}(z_4, z_2, z_1). \end{aligned} \quad (66)$$

With Eq. (56), one has

$$\begin{aligned} & \Sigma_{ij}^{(3),1,\{2;\{2;1,1\},0,B\}}(z_1, z_2) \\ &= (\mathrm{i}\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rs} \sum_{tv} w_{nsvt}(z_4) \\ & \quad \sum_u G_{tu}(z_4, z_2) \sum_w w_{uwjr}(z_2) G_{vw}(z_4, z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_4). \end{aligned} \quad (67)$$

For the third term, one finds

$$\begin{aligned} & \Sigma_{ij}^{(3),1,\{2;\{2;1,1\},0,C\}}(z_1, z_2) \\ &= \mathrm{i}\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),\{2;1,1\},0,C}(z_4, z_2, z_1). \end{aligned} \quad (68)$$

Employing Eq. (57), one arrives at

$$\begin{aligned} & \Sigma_{ij}^{(3),1,\{2;\{2;1,1\},0,C\}}(z_1, z_2) \\ &= (\mathrm{i}\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rs} \sum_{tv} w_{nvrt}(z_4) \\ & \quad \sum_u G_{tu}(z_4, z_2) \sum_w w_{usjw}(z_2) G_{vw}(z_2, z_4) G_{rp}(z_4, z_1) G_{qs}(z_1, z_2). \end{aligned} \quad (69)$$

1.3. Resummation approaches: GW approximation

The *GW* approximation solves Hedin’s equation for the screened interaction W according to Eq. (7) with the zeroth-order vertex $\Gamma^{(0)}$. The set of equations is given by the Dyson equation, cf. Eq. (1),

$$\begin{aligned} G_{ij}(z_1, z_2) &= G_{ij}^{(0)}(z_1, z_2) \\ &+ \int_C dz_3 dz_4 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \Sigma_{mn}(z_3, z_4) G_{nj}(z_4, z_2), \end{aligned} \quad (70)$$

the equation for the selfenergy [cf. Eq. (2)]

$$\Sigma_{ij}(z_1, z_2) = \Sigma_{ij}^H(z_1, z_2) + \Sigma_{ij}^{xc}(z_1, z_2), \quad (71)$$

with

$$\begin{aligned} \Sigma_{ij}^{xc}(z_1, z_2) &= \mathrm{i}\hbar \int_C dz_3 \sum_{mpq} W_{ipqm}(z_1, z_3) \\ & \quad \int_C dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(0)}(z_4, z_2, z_3) \\ &= \mathrm{i}\hbar \sum_{mp} W_{ipjm}(z_1, z_2) G_{mp}(z_1, z_2), \end{aligned} \quad (72)$$

the zeroth-order polarizability, cf. Eq. (14),

$$P_{ijkl}(z_1, z_2) = P_{ijkl}^{(0)}(z_1, z_2) = \pm i\hbar G_{ik}(z_1, z_2)G_{jl}(z_2, z_1), \quad (73)$$

the zeroth-order vertex, cf. Eq. (11),

$$\Gamma_{ijkl}(z_1, z_2, z_3) = \Gamma_{ijkl}^{(0)}(z_1, z_2, z_3) = \delta_C(z_1, z_{2+})\delta_C(z_3, z_2)\delta_{ik}\delta_{jl} \quad (74)$$

and the screened interaction [cf. Eqs. (5) and (7)]

$$W_{ijkl}(z_1, z_2) = \delta_C(z_1, z_2)w_{ijkl}(z_1) + W_{ijkl}^{\text{ns}}(z_1, z_2), \quad (75)$$

with

$$\begin{aligned} W_{ijkl}^{\text{ns}}(z_1, z_2) &= \sum_{mn} w_{imnl}(z_1) \int_C dz_3 \sum_{pq} P_{nqpm}^{(0)}(z_1, z_3) W_{pjkl}(z_3, z_2) \\ &= \pm i\hbar \sum_{mn} w_{imnl}(z_1) \int_C dz_3 \sum_{pq} G_{np}(z_1, z_3) G_{qm}(z_3, z_1) W_{pjkl}(z_3, z_2). \end{aligned} \quad (76)$$

To solve this set of equations, one has to determine the selfconsistent solution of Eq. (75). Thereto, it is more suitable to eliminate the singular bare interaction by using

$$\begin{aligned} W_{ijkl}^{\text{ns}}(z_1, z_2) &= W_{ijkl}(z_1, z_2) - W_{ijkl}^{\text{bare}}(z_1, z_2) \\ &= W_{ijkl}(z_1, z_2) - \delta_C(z_1, z_2)w_{ijkl}(z_1). \end{aligned} \quad (77)$$

The selfenergy [cf. Eqs. (71) and (72)] in terms of W^{ns} is then given by

$$\begin{aligned} \Sigma_{ij}^{\text{GW}}(z_1, z_2) &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + i\hbar \sum_{mp} W_{ipjm}(z_1, z_2)G_{mp}(z_1, z_2) \\ &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + i\hbar \sum_{mp} w_{ipjm}(z_1)G_{mp}(z_1, z_{1+})\delta_C(z_1, z_2) \\ &\quad + i\hbar \sum_{mp} W_{ipjm}^{\text{ns}}(z_1, z_2)G_{mp}(z_1, z_2). \end{aligned} \quad (78)$$

Using Eq. (10), the expression simplifies to

$$\begin{aligned} \Sigma_{ij}^{\text{GW}}(z_1, z_2) &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) + i\hbar \sum_{mp} W_{ipjm}^{\text{ns}}(z_1, z_2)G_{mp}(z_1, z_2) \\ &=: \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) + \Sigma_{ij}^{\text{GW,corr}}(z_1, z_2). \end{aligned} \quad (79)$$

For the screened interaction, one has

$$\begin{aligned} W_{ijkl}^{\text{ns}}(z_1, z_2) &= \pm i\hbar \sum_{mn} w_{imnl}(z_1) \sum_{pq} G_{np}(z_1, z_2) G_{qm}(z_2, z_1) w_{pjkl}(z_2) \\ &\quad \pm i\hbar \sum_{mn} w_{imnl}(z_1) \int_C dz_3 \sum_{pq} G_{np}(z_1, z_3) G_{qm}(z_3, z_1) W_{pjkl}^{\text{ns}}(z_3, z_2). \end{aligned} \quad (80)$$

1.4. Resummation approaches: T matrix

In contrast to the GW approximation, the T matrix is an approximation, which takes only the bare interaction w into account and aims instead at a good approximation of the bare vertex function Λ . Thus, its constitutive equations are the Dyson equation,

$$\begin{aligned} G_{ij}(z_1, z_2) &= \\ G_{ij}^{(0)}(z_1, z_2) + \int_C dz_3 dz_4 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \Sigma_{mn}(z_3, z_4) G_{nj}(z_4, z_2), \end{aligned} \quad (81)$$

the equation for the selfenergy, cf. Eqs. (2) and (3),

$$\Sigma_{ij}(z_1, z_2) = \Sigma_{ij}^H(z_1, z_2) + \Sigma_{ij}^{\text{xc}}(z_1, z_2), \quad (82)$$

with

$$\begin{aligned} \Sigma_{ij}^{\text{xc}}(z_1, z_2) &= \\ = i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_3 \sum_n G_{mn}(z_1, z_3) \Lambda_{nqpl}(z_3, z_2, z_1). \end{aligned} \quad (83)$$

The bare vertex Λ is self-consistently given as the solution of

$$\begin{aligned} \Lambda_{ijkl}(z_1, z_2, z_3) &= \delta_C(z_1, z_{2+}) \delta_C(z_3, z_2) \delta_{ik} \delta_{jl} \\ &\quad + \int_C dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_C dz_6 \sum_p G_{mp}(z_4, z_6) \\ &\quad \int_C dz_7 \sum_q G_{qn}(z_7, z_5) \Lambda_{pjkl}(z_6, z_7, z_3). \end{aligned} \quad (84)$$

If these equations are iterated ad infinitum, all selfenergy terms will be generated. To break the circular dependence between Eqs. (83) and (84), the T -matrix approximation starts by taking the bare vertex on the right-hand side of Eq. (84) only in zeroth order,

$$\Lambda_{ijkl}^{(0)}(z_1, z_2, z_3) = \delta_C(z_1, z_{2+}) \delta_C(z_3, z_2) \delta_{ik} \delta_{jl}, \quad (85)$$

transforming it into

$$\begin{aligned}\Lambda_{ijkl}^{\text{cl}}(z_1, z_2, z_3) &= \delta_C(z_1, z_{2+})\delta_C(z_3, z_2)\delta_{ik}\delta_{jl} \\ &+ \int_C dz_4 dz_5 \sum_{mn} \frac{\delta\Sigma_{il}^{\text{cl}}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} G_{mk}(z_4, z_3) G_{jn}(z_3, z_5).\end{aligned}\quad (86)$$

To arrive at a closed equation, this result is used in Eq. (82), yielding

$$\begin{aligned}\Sigma_{ij}^{\text{cl}}(z_1, z_2) &= \Sigma_{ij}^H(z_1, z_2) + \Sigma_{ij}^{\text{xc}}(z_1, z_2) \\ &= \Sigma_{ij}^H(z_1, z_2) + i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_3 \sum_n G_{mn}(z_1, z_3) \Lambda_{nqpj}^{\text{cl}}(z_3, z_2, z_1).\end{aligned}\quad (87)$$

Inserting Eq. (86), one has

$$\begin{aligned}\Sigma_{ij}^{\text{cl}}(z_1, z_2) &= \pm i\hbar \delta_C(z_1, z_2) \sum_{mn} w_{mijn}(z_1) G_{nm}(z_1, z_{1+}) \\ &+ i\hbar \sum_{mn} w_{injm}(z_1) G_{mn}(z_1, z_{1+}) \delta_C(z_1, z_2) \\ &+ i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\int_C dz_4 dz_5 \sum_{rs} \frac{\delta\Sigma_{nj}^{\text{cl}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5).\end{aligned}\quad (88)$$

This term can be restructured to yield

$$\begin{aligned}\Sigma_{ij}^{\text{cl}}(z_1, z_2) &= i\hbar \delta_C(z_1, z_2) \sum_{mn} G_{mn}(z_1, z_{1+}) w_{injm}^\pm(z_1) \\ &+ i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\int_C dz_4 dz_5 \sum_{rs} \frac{\delta\Sigma_{nj}^{\text{cl}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5),\end{aligned}\quad (89)$$

with the (anti-)symmetrized potential $w_{ijkl}^\pm(z_1) := w_{ijkl}(z_1) \pm w_{jikl}(z_1)$. Using Eq. (10) again, one finds

$$\begin{aligned}\Sigma_{ij}^{\text{cl}}(z_1, z_2) &= \Sigma_{ij}^H(z_1, z_2) + \Sigma_{ij}^F(z_1, z_2) + i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\int_C dz_4 dz_5 \sum_{rs} \frac{\delta\Sigma_{nj}^{\text{cl}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5).\end{aligned}\quad (90)$$

Taking the derivative with respect to G , one arrives at

$$\begin{aligned} \frac{\delta \Sigma_{ij}^{\text{cl}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} &= i\hbar \delta_C(z_1, z_2) \delta_C(z_1, z_6) \delta_C(z_{1+}, z_7) w_{iujt}^\pm(z_1) \\ &\left(\frac{\delta \Sigma_{ij}^{\text{cl,A}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} + \frac{\delta \Sigma_{ij}^{\text{cl,B}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \right. \\ &\left. + \frac{\delta \Sigma_{ij}^{\text{cl,C}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} + \frac{\delta \Sigma_{ij}^{\text{cl,D}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \right), \end{aligned} \quad (91)$$

with

$$\begin{aligned} \frac{\delta \Sigma_{ij}^{\text{cl,A}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} &= i\hbar \delta_C(z_1, z_6) \sum_{pq} w_{ipqt}(z_1) \\ &\int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{uj}^{\text{cl}}(z_7, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5), \end{aligned} \quad (92)$$

$$\begin{aligned} \frac{\delta \Sigma_{ij}^{\text{cl,B}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} &= i\hbar \delta_C(z_1, z_7) \sum_{mq} w_{iuqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\int_{\mathcal{C}} dz_5 \sum_s \frac{\delta \Sigma_{nj}^{\text{cl}}(z_3, z_2)}{\delta G_{ts}(z_6, z_5)} G_{qs}(z_1, z_5) \end{aligned} \quad (93)$$

and

$$\begin{aligned} \frac{\delta \Sigma_{ij}^{\text{cl,C}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} &= i\hbar \delta_C(z_1, z_6) \sum_{mp} w_{iptm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\int_{\mathcal{C}} dz_4 \sum_r \frac{\delta \Sigma_{nj}^{\text{cl}}(z_3, z_2)}{\delta G_{ru}(z_4, z_7)} G_{rp}(z_4, z_1), \end{aligned} \quad (94)$$

as well as

$$\begin{aligned} & \frac{\delta \Sigma_{ij}^{\text{cl,D}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \\ &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_3 \sum_n G_{mn}(z_1, z_3) \\ & \quad \int_C dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{nj}^{\text{cl}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5) \delta G_{tu}(z_6, z_7)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5). \end{aligned} \quad (95)$$

Neglecting $\frac{\delta \Sigma_{nj}^{\text{cl}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5) \delta G_{tu}(z_6, z_7)}$ as an approximation, Eq. (91) becomes a closed equation for $\frac{\delta \Sigma^{\text{cl}}}{\delta G}$. The first iteration yields the second-order terms

$$\begin{aligned} & \frac{\delta \Sigma_{ij}^{\text{cl},(2)}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \approx \frac{\delta \Sigma_{ij}^{\text{cl},(2),A}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \\ & \quad + \frac{\delta \Sigma_{ij}^{\text{cl},(2),B}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} + \frac{\delta \Sigma_{ij}^{\text{cl},(2),C}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)}, \end{aligned} \quad (96)$$

with

$$\begin{aligned} & \frac{\delta \Sigma_{ij}^{\text{cl},(2),A}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \\ &= (i\hbar)^2 \delta_C(z_1, z_6) \delta_C(z_2, z_7) \sum_{pq} w_{ipqt}(z_1) \\ & \quad \sum_{rs} w_{usjr}^\pm(z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_2) \end{aligned} \quad (97)$$

and

$$\begin{aligned} & \frac{\delta \Sigma_{ij}^{\text{cl},(2),B}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \\ &= (i\hbar)^2 \delta_C(z_1, z_7) \delta_C(z_2, z_6) \sum_{mq} w_{iuqm}(z_1) \\ & \quad \sum_n G_{mn}(z_1, z_2) \sum_s w_{nsjt}^\pm(z_2) G_{qs}(z_1, z_2) \end{aligned} \quad (98)$$

as well as

$$\begin{aligned} & \frac{\delta \Sigma_{ij}^{\text{cl},(2),C}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \\ &= (i\hbar)^2 \delta_C(z_1, z_6) \delta_C(z_2, z_7) \sum_{mp} w_{iptm}(z_1) \\ & \quad \sum_n G_{mn}(z_1, z_2) \sum_r w_{nujr}^\pm(z_2) G_{rp}(z_2, z_1). \end{aligned} \quad (99)$$

Note that, for the first iteration, $\frac{\delta \Sigma_{ij}^{\text{cl},\text{D}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)}$ is exactly equal to zero, thus Eq. (96) is also exact up to second order in w . In the following, each of the three terms will be considered separately. To start with, one recognizes that all three terms yield the same first and second-order contributions to the selfenergy, which read

$$\Sigma_{ij}^{\text{cl},(1)}(z_1, z_2) = \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) \quad (100)$$

$$\Sigma_{ij}^{\text{cl},(2)}(z_1, z_2) = (\text{i}\hbar)^2 \sum_{mpq} w_{ipqm}(z_1) \sum_n G_{mn}(z_1, z_2) \quad (101)$$

$$\sum_{rs} w_{nsjr}^\pm(z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_2)$$

and agree with the exact first and second-order terms, already encountered in Eqs. (9), (18) and (27). The third-order contributions to Σ^{cl} from the second-order terms in Eq. (96) are given by

$$\begin{aligned} \Sigma_{ij}^{\text{cl},(3),\text{A}}(z_1, z_2) &= \text{i}\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\quad \int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{nj}^{\text{cl},(2),\text{A}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5). \end{aligned} \quad (102)$$

Inserting the second-order term yields

$$\begin{aligned} \Sigma_{ij}^{\text{cl},(3),\text{A}}(z_1, z_2) &= (\text{i}\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\quad \sum_{rs} \sum_{tu} w_{ntur}(z_3) \sum_{vw} w_{swjv}^\pm(z_2) \\ &\quad G_{vt}(z_2, z_3) G_{uw}(z_3, z_2) G_{rp}(z_3, z_1) G_{qs}(z_1, z_2). \end{aligned} \quad (103)$$

For the second third-order selfenergy term, one has

$$\begin{aligned} \Sigma_{ij}^{\text{cl},(3),\text{B}}(z_1, z_2) &= \text{i}\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\quad \int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{nj}^{\text{cl},(2),\text{B}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5). \end{aligned} \quad (104)$$

which evaluates to

$$\begin{aligned} \Sigma_{ij}^{\text{cl},(3),\text{B}}(z_1, z_2) &= (\text{i}\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\quad \sum_{rs} \sum_{tu} w_{nsut}(z_3) \sum_v G_{tv}(z_3, z_2) \sum_w w_{vwjr}^\pm(z_2) \\ &\quad G_{uw}(z_3, z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_3). \end{aligned} \quad (105)$$

The third term reads

$$\Sigma_{ij}^{\text{cl},(3),\text{C}}(z_1, z_2) = i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \quad (106)$$

$$\int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{nj}^{\text{cl},(2),\text{C}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5). \quad (107)$$

Using the second-order result, one arrives at

$$\begin{aligned} \Sigma_{ij}^{\text{cl},(3),\text{C}}(z_1, z_2) &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\quad \sum_{rs} \sum_{tu} w_{nurt}(z_3) \sum_v G_{tv}(z_3, z_2) \sum_w w_{vsjw}^\pm(z_2) \\ &\quad G_{wu}(z_2, z_3) G_{rp}(z_3, z_1) G_{qs}(z_1, z_2). \end{aligned} \quad (108)$$

2. Non-selfconsistent second-order selfenergy contributions

2.1. General basis

The first two classes are just the same as in the selfconsistent approximation, cf. Eqs. (176) and (183) of the main text, with the replacement $G \rightarrow G^{(0)}$. Likewise, their components follow directly from Eqs. (184) and (185) of the main text. For the third and fourth class, one needs the contributions to $G^{(1)}$, which are

$$\begin{aligned} G_{ij}^{(1),\{\text{H},0\},0}(z_1, z_2) &= \int_{\mathcal{C}} dz_3 dz_4 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \Sigma_{mn}^{\text{H},0}(z_3, z_4) G_{nj}^{(0)}(z_4, z_2) \\ &= \pm i\hbar \int_{\mathcal{C}} dz_3 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \sum_{pq} w_{pmnq}(z_3) G_{qp}^{(0)}(z_3, z_{3+}) G_{nj}^{(0)}(z_3, z_2) \end{aligned} \quad (109)$$

and

$$\begin{aligned} G_{ij}^{(1),\{\text{F},0\},0}(z_1, z_2) &= \int_{\mathcal{C}} dz_3 dz_4 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \Sigma_{mn}^{\text{F},0}(z_3, z_4) G_{nj}^{(0)}(z_4, z_2) \\ &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \sum_{pq} w_{mqnp}(z_3) G_{pq}^{(0)}(z_3, z_{3+}) G_{nj}^{(0)}(z_3, z_2). \end{aligned} \quad (110)$$

With these results, the additional non-selfconsistent contributions are

$$\begin{aligned} \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\}}(z_1, z_2) &= \pm i\hbar\delta_C(z_1, z_2) \sum_{mn} w_{mijn}(z_1) G_{nm}^{(1),\{\text{H},0\},0}(z_1, z_{1+}) \\ &= (i\hbar)^2 \delta_C(z_1, z_2) \sum_{mn} w_{mijn}(z_1) \\ &\quad \int_C dz_3 \sum_{pq} G_{np}^{(0)}(z_1, z_3) \sum_{rs} w_{rpqs}(z_3) G_{sr}^{(0)}(z_3, z_{3+}) G_{qm}^{(0)}(z_3, z_{1+}), \end{aligned} \quad (111)$$

as well as

$$\begin{aligned} \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\}}(z_1, z_2) &= \pm i\hbar\delta_C(z_1, z_2) \sum_{mn} w_{mijn}(z_1) G_{nm}^{(1),\{\text{F},0\},0}(z_1, z_{1+}) \\ &= \pm (i\hbar)^2 \delta_C(z_1, z_2) \sum_{mn} w_{mijn}(z_1) \\ &\quad \int_C dz_3 \sum_{pq} G_{np}^{(0)}(z_1, z_3) \sum_{rs} w_{psqr}(z_3) G_{rs}^{(0)}(z_3, z_{3+}) G_{qm}^{(0)}(z_3, z_{1+}) \end{aligned} \quad (112)$$

and

$$\begin{aligned} \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\}}(z_1, z_2) &= i\hbar\delta_C(z_1, z_2) \sum_{mn} w_{injm}(z_1) G_{mn}^{(1),\{\text{H},0\},0}(z_1, z_{1+}) \\ &= \pm (i\hbar)^2 \delta_C(z_1, z_2) \sum_{mn} w_{nimj}(z_1) \\ &\quad \int_C dz_3 \sum_{pq} G_{mp}^{(0)}(z_1, z_3) \sum_{rs} w_{rpqs}(z_3) G_{sr}^{(0)}(z_3, z_{3+}) G_{qn}^{(0)}(z_3, z_{1+}), \end{aligned} \quad (113)$$

as well as

$$\begin{aligned} \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\}}(z_1, z_2) &= i\hbar\delta_C(z_1, z_2) \sum_{mn} w_{injm}(z_1) G_{mn}^{(1),\{\text{F},0\},0}(z_1, z_{1+}) \\ &= (i\hbar)^2 \delta_C(z_1, z_2) \sum_{mn} w_{nimj}(z_1) \\ &\quad \int_C dz_3 \sum_{pq} G_{mp}^{(0)}(z_1, z_3) \sum_{rs} w_{psqr}(z_3) G_{rs}^{(0)}(z_3, z_{3+}) G_{qn}^{(0)}(z_3, z_{1+}). \end{aligned} \quad (114)$$

The corresponding components are all time-diagonal and read

$$\begin{aligned} \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\delta}(t_1) &= (i\hbar)^2 \sum_{mn} w_{mijn}(t_1) \left(\right. \\ &\quad \int_{t_0}^{t_1} dt_3 \sum_{pq} G_{np}^{(0),>}(t_1, t_3) \sum_{rs} w_{rpqs}(t_3) G_{sr}^{(0),<}(t_3, t_3) G_{qm}^{(0),<}(t_3, t_1) \\ &\quad \left. + \int_{t_1}^{t_0} dt_3 \sum_{pq} G_{np}^{(0),<}(t_1, t_3) \sum_{rs} w_{rpqs}(t_3) G_{sr}^{(0),<}(t_3, t_3) G_{qm}^{(0),>}(t_3, t_1) \right) \end{aligned} \quad (115)$$

and

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\},\delta}(t_1) \\ &= \pm (\text{i}\hbar)^2 \sum_{mn} w_{mijn}(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_{pq} G_{np}^{(0),>}(t_1, t_3) \sum_{rs} w_{psqr}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{qm}^{(0),<}(t_3, t_1) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_{pq} G_{np}^{(0),<}(t_1, t_3) \sum_{rs} w_{psqr}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{qm}^{(0),>}(t_3, t_1) \right), \end{aligned} \quad (116)$$

as well as

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\},\delta}(t_1) \\ &= \pm (\text{i}\hbar)^2 \sum_{mn} w_{nimj}(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_{pq} G_{mp}^{(0),>}(t_1, t_3) \sum_{rs} w_{rpqs}(t_3) G_{sr}^{(0),<}(t_3, t_3) G_{qn}^{(0),<}(t_3, t_1) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_{pq} G_{mp}^{(0),<}(t_1, t_3) \sum_{rs} w_{rpqs}(t_3) G_{sr}^{(0),<}(t_3, t_3) G_{qn}^{(0),>}(t_3, t_1) \right) \end{aligned} \quad (117)$$

and

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\},\delta}(t_1) \\ &= (\text{i}\hbar)^2 \sum_{mn} w_{nimj}(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_{pq} G_{mp}^{(0),>}(t_1, t_3) \sum_{rs} w_{psqr}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{qn}^{(0),<}(t_3, t_1) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_{pq} G_{mp}^{(0),<}(t_1, t_3) \sum_{rs} w_{psqr}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{qn}^{(0),>}(t_3, t_1) \right). \end{aligned} \quad (118)$$

2.2. Diagonal basis

For $w_{ijkl} = \delta_{il}\delta_{jk}w_{ij}$, the non-selfconsistent selfenergy terms attain the form, cf. Eqs. (189) and (191) of the main text,

$$\begin{aligned} & \Sigma_{ij}^{(2),(2),2,0,0,\text{diagonal}}(z_1, z_2) \\ & \equiv \Sigma_{ij}^{(2),2,0,\text{diagonal}}(z_1, z_2)(G \rightarrow G^{(0)}) \end{aligned} \quad (119)$$

and

$$\begin{aligned} & \Sigma_{ij}^{(2),(2),1,0,1,\text{diagonal}}(z_1, z_2) \\ & \equiv \Sigma_{ij}^{(2),1,1,\text{diagonal}}(z_1, z_2)(G \rightarrow G^{(0)}), \end{aligned} \quad (120)$$

as well as

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{diagonal}}(z_1, z_2) \\ &= (\text{i}\hbar)^2 \delta_C(z_1, z_2) \delta_{ij} \sum_m w_{mi}(z_1) \\ & \quad \int_C dz_3 \sum_p G_{mp}^{(0)}(z_1, z_3) G_{pm}^{(0)}(z_3, z_{1+}) \sum_r w_{rp}(z_3) G_{rr}^{(0)}(z_3, z_{3+}) \end{aligned} \quad (121)$$

and

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\},\text{diagonal}}(z_1, z_2) \\ &= \pm (\text{i}\hbar)^2 \delta_C(z_1, z_2) \delta_{ij} \sum_m w_{mi}(z_1) \\ & \quad \int_C dz_3 \sum_p G_{mp}^{(0)}(z_1, z_3) \sum_q w_{pq}(z_3) G_{pq}^{(0)}(z_3, z_{3+}) G_{qm}^{(0)}(z_3, z_{1+}). \end{aligned} \quad (122)$$

Further,

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\},\text{diagonal}}(z_1, z_2) \\ &= \pm (\text{i}\hbar)^2 \delta_C(z_1, z_2) w_{ij}(z_1) \\ & \quad \int_C dz_3 \sum_p G_{ip}^{(0)}(z_1, z_3) \sum_r w_{rp}(z_3) G_{rr}^{(0)}(z_3, z_{3+}) G_{pj}^{(0)}(z_3, z_{1+}) \end{aligned} \quad (123)$$

and

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\},\text{diagonal}}(z_1, z_2) \\ &= (\text{i}\hbar)^2 \delta_C(z_1, z_2) w_{ij}(z_1) \\ & \quad \int_C dz_3 \sum_p G_{ip}^{(0)}(z_1, z_3) \sum_q w_{pq}(z_3) G_{pq}^{(0)}(z_3, z_{3+}) G_{qj}^{(0)}(z_3, z_{1+}). \end{aligned} \quad (124)$$

The components read [cf. Eqs. (191) and (192) of the main text]

$$\Sigma_{ij}^{(2),(2),2,0,0,\text{diagonal},\gtrless}(t_1, t_2) \equiv \Sigma_{ij}^{(2),2,0,\text{diagonal},\gtrless}(t_1, t_2)(G \rightarrow G^{(0)}), \quad (125)$$

$$\Sigma_{ij}^{(2),(2),1,0,1,\text{diagonal},\gtrless}(t_1, t_2) \equiv \Sigma_{ij}^{(2),1,1,\text{diagonal},\gtrless}(t_1, t_2)(G \rightarrow G^{(0)}), \quad (126)$$

as well as [cf. Eq. (115) to Eq. (119)]

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{diagonal},\delta}(t_1) \\ &= (\text{i}\hbar)^2 \delta_{ij} \sum_m w_{mi}(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{mp}^{(0),>}(t_1, t_3) \sum_r w_{rp}(t_3) G_{rr}^{(0),<}(t_3, t_3) G_{pm}^{(0),<}(t_3, t_1) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{mp}^{(0),<}(t_1, t_3) \sum_r w_{rp}(t_3) G_{rr}^{(0),<}(t_3, t_3) G_{pm}^{(0),>}(t_3, t_1) \right) \end{aligned} \quad (127)$$

and

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\},\delta}(t_1) \\ &= \pm (\text{i}\hbar)^2 \delta_{ij} \sum_m w_{mi}(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 G_{mr}^{(0),>}(t_1, t_3) \sum_{rs} w_{rs}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{sm}^{(0),<}(t_3, t_1) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 G_{mr}^{(0),<}(t_1, t_3) \sum_{rs} w_{rs}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{sm}^{(0),>}(t_3, t_1) \right). \end{aligned} \quad (128)$$

Further,

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\},\text{diagonal},\delta}(t_1, t_2) \\ &= \pm (\text{i}\hbar)^2 w_{ji}(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{ip}^{(0),>}(t_1, t_3) \sum_{rs} w_{rp}(t_3) G_{rr}^{(0),<}(t_3, t_3) G_{pj}^{(0),<}(t_3, t_1) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{ip}^{(0),<}(t_1, t_3) \sum_{rs} w_{rp}(t_3) G_{rr}^{(0),<}(t_3, t_3) G_{pj}^{(0),>}(t_3, t_1) \right) \end{aligned} \quad (129)$$

and

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\},\delta}(t_1) \\ &= (\text{i}\hbar)^2 \sum_n w_{ji}(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 G_{ir}^{(0),<}(t_1, t_3) \sum_{rs} w_{rs}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{sj}^{(0),>}(t_3, t_1) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 G_{ir}^{(0),>}(t_1, t_3) \sum_{rs} w_{rs}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{sj}^{(0),<}(t_3, t_1) \right). \end{aligned} \quad (130)$$

2.3. Hubbard basis

In the Hubbard basis, the non-selfconsistent contributions attain the form

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard},\mathfrak{b}}(z_1, z_2) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard},\mathfrak{b}}(z_1, z_2)(G \rightarrow G^{(0)}) \end{aligned} \quad (131)$$

and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard},\mathfrak{b}}(z_1, z_2) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard},\mathfrak{b}}(z_1, z_2)(G \rightarrow G^{(0)}), \end{aligned} \quad (132)$$

as well as

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{b}}(z_1, z_2) \\ &= (\mathrm{i}\hbar)^2 \delta_C(z_1, z_2) \delta_{ij} \sum_{\epsilon} U(z_1) \\ & \quad \int_C dz_3 \sum_p G_{i\epsilon p\epsilon}^{(0)}(z_1, z_3) G_{p\epsilon i\epsilon}^{(0)}(z_3, z_{1+}) \sum_{\zeta} U(z_3) G_{p\zeta p\zeta}^{(0)}(z_3, z_{3+}) \end{aligned} \quad (133)$$

and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\},\text{Hubbard},\mathfrak{b}}(z_1, z_2) \\ &= (\mathrm{i}\hbar)^2 \delta_C(z_1, z_2) \delta_{ij} \sum_{\epsilon} U(z_1) \\ & \quad \int_C dz_3 \sum_p G_{i\epsilon p\epsilon}^{(0)}(z_1, z_3) U(z_3) G_{p\epsilon p\epsilon}^{(0)}(z_3, z_{3+}) G_{p\epsilon i\epsilon}^{(0)}(z_3, z_{1+}). \end{aligned} \quad (134)$$

Further,

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{b}}(z_1, z_2) \\ &= (\mathrm{i}\hbar)^2 \delta_C(z_1, z_2) \delta_{ij} U(z_1) \\ & \quad \int_C dz_3 \sum_p G_{i\alpha p\alpha}^{(0)}(z_1, z_3) U(z_3) \sum_{\epsilon} G_{p\epsilon p\epsilon}^{(0)}(z_3, z_{3+}) G_{p\alpha i\alpha}^{(0)}(z_3, z_{1+}) \end{aligned} \quad (135)$$

and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\},\text{Hubbard},\mathfrak{b}}(z_1, z_2) \\ &= (\mathrm{i}\hbar)^2 \delta_C(z_1, z_2) \delta_{ij} U(z_1) \\ & \quad \int_C dz_3 \sum_p G_{i\alpha p\alpha}^{(0)}(z_1, z_3) U(z_3) G_{p\alpha p\alpha}^{(0)}(z_1, z_{1+}) G_{p\alpha i\alpha}^{(0)}(z_3, z_{1+}), \end{aligned} \quad (136)$$

for bosons, and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard},\mathfrak{f}}(z_1, z_2) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard},\mathfrak{f}}(z_1, z_2) (G \rightarrow G^{(0)}) \end{aligned} \quad (137)$$

and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard},\mathfrak{f}}(z_1, z_2) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard},\mathfrak{f}}(z_1, z_2) (G \rightarrow G^{(0)}), \end{aligned} \quad (138)$$

as well as

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{f}}(z_1, z_2) \\ &= (\mathrm{i}\hbar)^2 \delta_C(z_1, z_2) \delta_{ij} \sum_{\epsilon \neq \alpha} U(z_1) \end{aligned} \quad (139)$$

$$\begin{aligned} & \int_C dz_3 \sum_p G_{i\epsilon p\epsilon}^{(0)}(z_1, z_3) G_{p\epsilon i\epsilon}^{(0)}(z_3, z_{1+}) \sum_{\zeta \neq \epsilon} U(z_3) G_{p\zeta p\zeta}^{(0)}(z_3, z_{3+}), \\ & \Sigma_{i\alpha j\alpha}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\},\text{Hubbard},\mathfrak{f}}(z_1, z_2) \equiv 0 \end{aligned} \quad (140)$$

and

$$\Sigma_{i\alpha j\alpha}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{f}}(z_1, z_2) \equiv 0, \quad (141)$$

$$\Sigma_{i\alpha j\alpha}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\},\text{Hubbard},\mathfrak{f}}(z_1, z_2) \equiv 0, \quad (142)$$

for fermions. The components read

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard},\mathfrak{b},\gtrless}(t_1, t_2) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard},\mathfrak{b},\gtrless}(t_1, t_2)(G \rightarrow G^{(0)}) , \end{aligned} \quad (143)$$

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard},\mathfrak{b},\gtrless}(t_1, t_2) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard},\mathfrak{b},\gtrless}(t_1, t_2)(G \rightarrow G^{(0)}) , \end{aligned} \quad (144)$$

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard},\mathfrak{f},\gtrless}(t_1, t_2) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard},\mathfrak{f},\gtrless}(t_1, t_2)(G \rightarrow G^{(0)}) , \end{aligned} \quad (145)$$

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard},\mathfrak{f},\gtrless}(t_1, t_2) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard},\mathfrak{f},\gtrless}(t_1, t_2)(G \rightarrow G^{(0)}) , \end{aligned} \quad (146)$$

as well as

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{b},\delta}(t_1, t_2) \\ &= (\mathrm{i}\hbar)^2 \delta_{ij} \sum_{\epsilon} U(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),>}(t_1, t_3) G_{p\epsilon i\epsilon}^{(0),<}(t_3, t_1) \sum_{\zeta} U(t_3) G_{p\zeta p\zeta}^{(0),<}(t_3, t_3) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),<}(t_1, t_3) G_{p\epsilon i\epsilon}^{(0),>}(t_3, t_1) \sum_{\zeta} U(t_3) G_{p\zeta p\zeta}^{(0),<}(t_3, t_3) \right) \end{aligned} \quad (147)$$

and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\},\text{Hubbard},\mathfrak{b},\delta}(t_1, t_2) \\ &= (\mathrm{i}\hbar)^2 \delta_{ij} \sum_{\epsilon} U(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),>}(t_1, t_3) U(t_3) G_{p\epsilon p\epsilon}^{(0),<}(t_3, t_3) G_{p\epsilon i\alpha}^{(0),<}(t_3, t_1) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),<}(t_1, t_3) U(t_3) G_{p\epsilon p\epsilon}^{(0),<}(t_3, t_3) G_{p\epsilon i\epsilon}^{(0),>}(t_3, t_1) \right). \end{aligned} \quad (148)$$

Further,

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{b},\delta}(t_1, t_2) \\ &= (\mathrm{i}\hbar)^2 \delta_{ij} U(z_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{i\alpha p\alpha}^{(0),>}(t_1, t_3) U(t_3) \sum_{\epsilon} G_{p\epsilon p\epsilon}^{(0),<}(t_3, t_3) G_{p\alpha i\alpha}^{(0),<}(t_3, t_1) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\alpha p\alpha}^{(0),<}(t_1, t_3) U(t_3) \sum_{\epsilon} G_{p\epsilon p\epsilon}^{(0),<}(t_3, t_3) G_{p\alpha i\alpha}^{(0),>}(t_3, t_1) \right) \end{aligned} \quad (149)$$

and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\},\text{Hubbard},\mathfrak{b},\delta}(t_1, t_2) \\ &= (\mathrm{i}\hbar)^2 \delta_{ij} U(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{i\alpha p\alpha}^{(0),>}(t_1, t_3) U(t_3) G_{p\alpha p\alpha}^{(0),<}(t_3, t_3) G_{p\alpha i\alpha}^{(0),<}(t_3, t_1) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\alpha p\alpha}^{(0),<}(t_1, t_3) U(t_3) G_{p\alpha p\alpha}^{(0),<}(t_3, t_3) G_{p\alpha i\alpha}^{(0),>}(t_3, t_1) \right) \end{aligned} \quad (150)$$

and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{f},\delta}(t_1, t_2) \\ &= (\mathrm{i}\hbar)^2 \delta_{ij} \sum_{\epsilon \neq \alpha} U(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),>}(t_1, t_3) G_{p\epsilon i\epsilon}^{(0),<}(t_3, t_1) \sum_{\zeta \neq \epsilon} U(t_3) G_{p\zeta p\zeta}^{(0),<}(t_3, t_3) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),<}(t_1, t_3) G_{p\epsilon i\epsilon}^{(0),>}(t_3, t_1) \sum_{\zeta \neq \epsilon} U(t_3) G_{p\zeta p\zeta}^{(0),<}(t_3, t_3) \right). \end{aligned} \quad (151)$$

2.4. Spin-0 bosons/spin-1/2 fermions

For the specific bosonic and fermionic cases, one has

$$\begin{aligned} & \Sigma_{ij}^{(2),(2),2,0,0,\text{Hubbard},\mathfrak{b},0}(z_1, z_2) \\ & \equiv \Sigma_{ij}^{(2),2,0,\text{Hubbard},\mathfrak{b},0}(z_1, z_2)(G \rightarrow G^{(0)}) \end{aligned} \quad (152)$$

and

$$\begin{aligned} & \Sigma_{ij}^{(2),(2),1,0,1,\text{Hubbard},\mathfrak{b},0}(z_1, z_2) \\ & \equiv \Sigma_{ij}^{(2),1,1,\text{Hubbard},\mathfrak{b},0}(z_1, z_2)(G \rightarrow G^{(0)}) , \end{aligned} \quad (153)$$

as well as

$$\begin{aligned} & \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{b},0}(z_1, z_2) \\ & = \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\},\text{Hubbard},\mathfrak{b},0}(z_1, z_2) \\ & = \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{b},0}(z_1, z_2) \\ & = \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\},\text{Hubbard},\mathfrak{b},0}(z_1, z_2) \\ & = (\mathrm{i}\hbar)^2 \delta_C(z_1, z_2) \delta_{ij} U(z_1) \\ & \quad \int_C dz_3 \sum_p G_{ip}^{(0)}(z_1, z_3) G_{pi}^{(0)}(z_3, z_{1+}) U(z_3) G_{pp}^{(0)}(z_3, z_{3+}) , \end{aligned} \quad (154)$$

for spin-0 bosons, and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard},\mathfrak{f},1/2}(z_1, z_2) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard},\mathfrak{f},1/2}(z_1, z_2)(G \rightarrow G^{(0)}) \end{aligned} \quad (155)$$

and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard},\mathfrak{f},1/2}(z_1, z_2) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard},\mathfrak{f},1/2}(z_1, z_2)(G \rightarrow G^{(0)}) , \end{aligned} \quad (156)$$

as well as

$$\begin{aligned} & \Sigma_{i\uparrow j\uparrow}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{f},1/2}(z_1, z_2) \\ & = (\mathrm{i}\hbar)^2 \delta_C(z_1, z_2) \delta_{ij} U(z_1) \\ & \quad \int_C dz_3 \sum_p G_{i\downarrow p\downarrow}^{(0)}(z_1, z_3) G_{p\downarrow i\downarrow}^{(0)}(z_3, z_{1+}) U(z_3) G_{p\uparrow p\uparrow}^{(0)}(z_3, z_{3+}) \end{aligned} \quad (157)$$

and

$$\begin{aligned} \Sigma_{i\downarrow j\downarrow}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{f},1/2}(z_1, z_2) \\ = (\mathrm{i}\hbar)^2 \delta_C(z_1, z_2) \delta_{ij} U(z_1) \\ \int_C dz_3 \sum_p G_{i\uparrow p\uparrow}^{(0)}(z_1, z_3) G_{p\uparrow i\uparrow}^{(0)}(z_3, z_{1+}) U(z_3) G_{p\downarrow p\downarrow}^{(0)}(z_3, z_{3+}), \end{aligned} \quad (158)$$

for spin-1/2 fermions. The corresponding components read

$$\begin{aligned} \Sigma_{ij}^{(2),(2),2,0,0,\text{Hubbard},\mathfrak{b},0,\gtrless}(t_1, t_2) \\ \equiv \Sigma_{ij}^{(2),2,0,\text{Hubbard},\mathfrak{b},0,\gtrless}(t_1, t_2) (G \rightarrow G^{(0)}) , \end{aligned} \quad (159)$$

$$\begin{aligned} \Sigma_{ij}^{(2),(2),1,0,1,\text{Hubbard},\mathfrak{b},0,\gtrless}(t_1, t_2) \\ \equiv \Sigma_{ij}^{(2),1,1,\text{Hubbard},\mathfrak{b},0,\gtrless}(t_1, t_2) (G \rightarrow G^{(0)}) , \end{aligned} \quad (160)$$

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard},\mathfrak{f},1/2,\gtrless}(t_1, t_2) \\ \equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard},\mathfrak{f},1/2,\gtrless}(t_1, t_2) (G \rightarrow G^{(0)}) , \end{aligned} \quad (161)$$

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard},\mathfrak{f},1/2,\gtrless}(t_1, t_2) \\ \equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard},\mathfrak{f},1/2,\gtrless}(t_1, t_2) (G \rightarrow G^{(0)}) , \end{aligned} \quad (162)$$

as well as

$$\begin{aligned} \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{b},0,\delta}(t_1, t_2) \\ = \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\},\text{Hubbard},\mathfrak{b},0,\delta}(t_1, t_2) \\ = \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{b},0,\delta}(t_1, t_2) \\ = \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\},\text{Hubbard},\mathfrak{b},0,\delta}(t_1, t_2) \\ = (\mathrm{i}\hbar)^2 \delta_{ij} U(t_1) \left(\right. \\ \left. \int_{t_0}^{t_1} dt_3 \sum_p G_{ip}^{(0),>}(t_1, t_3) G_{pi}^{(0),<}(t_3, t_1) U(t_3) G_{pp}^{(0),<}(t_3, t_3) \right. \\ \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{ip}^{(0),<}(t_1, t_3) G_{pi}^{(0),>}(t_3, t_1) U(t_3) G_{pp}^{(0),<}(t_3, t_3) \right) , \end{aligned} \quad (163)$$

for spin-0 bosons, and

$$\begin{aligned} & \Sigma_{i\uparrow j\uparrow}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{f},1/2,\delta}(t_1, t_2) \\ &= (\mathrm{i}\hbar)^2 \delta_{ij} U(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{i\downarrow p\downarrow}^{(0),>}(t_1, t_3) G_{p\downarrow i\downarrow}^{(0),<}(t_3, t_1) U(t_3) G_{p\uparrow p\uparrow}^{(0),<}(t_3, t_3) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\downarrow p\downarrow}^{(0),<}(t_1, t_3) G_{p\downarrow i\downarrow}^{(0),>}(t_3, t_1) U(t_3) G_{p\uparrow p\uparrow}^{(0),<}(t_3, t_3) \right), \end{aligned} \quad (164)$$

as well as

$$\begin{aligned} & \Sigma_{i\downarrow j\downarrow}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard},\mathfrak{f},1/2,\delta}(t_1, t_2) \\ &= (\mathrm{i}\hbar)^2 \delta_{ij} U(t_1) \left(\right. \\ & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{i\uparrow p\uparrow}^{(0),>}(t_1, t_3) G_{p\uparrow i\uparrow}^{(0),<}(t_3, t_1) U(t_3) G_{p\downarrow p\downarrow}^{(0),<}(t_3, t_3) \\ & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\uparrow p\uparrow}^{(0),<}(t_1, t_3) G_{p\uparrow i\uparrow}^{(0),>}(t_3, t_1) U(t_3) G_{p\downarrow p\downarrow}^{(0),<}(t_3, t_3) \right), \end{aligned} \quad (165)$$

for spin-1/2 fermions.