Computation Of Green's Functions From Dyson's Equation With Self-Energy Evaluated Through Second Order

Homer Reid

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1 Overview

2 Notation And Conventions

2.1 The Hamiltonian

We work in a basis ϕ_α of eigenstates of the noninteracting Hamiltonian,

$$H_0 = \sum E_\alpha a_\alpha^\dagger a_\alpha.$$

Then the perturbation is

$$V = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$$

where

$$V_{\alpha\beta\gamma\delta} = \int d\mathbf{r}\, d\mathbf{r}' \phi_\alpha^*(\mathbf{r})\phi_\beta^*(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\phi_\gamma(\mathbf{r})\phi_\delta(\mathbf{r}')$$

where $V(\mathbf{r},\mathbf{r}') = \frac{1}{|\mathbf{r}-\mathbf{r}'|}$ in our case.

2.2 The Green's Functions

The object we seek to compute is

$$\begin{aligned} iG_{\alpha\beta}(t) &= \Big\langle \Omega \Big| T a_\alpha(t) a_\beta^\dagger(0) \Big| \Omega \Big\rangle \\ &= \begin{cases} \Big\langle \Omega \Big| a_\alpha(t) a_\beta^\dagger(0) \Big| \Omega \Big\rangle, & t > 0 \\ -\Big\langle \Omega \Big| a_\beta^\dagger(0) a_\alpha(t) \Big| \Omega \Big\rangle, & t < 0, \end{cases} \end{aligned}$$

where $|\Omega\rangle$ is the ground state of the interacting system.

For the Fourier representation we use the (backwards, in my view, but standard) conventions

$$iG_{\alpha\beta}(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} iG_{\alpha\beta}(\omega), \qquad iG_{\alpha\beta}(\omega) = \int dt\, e^{+i\omega t} iG_{\alpha\beta}(t).$$

The noninteracting Green's function is

$$iG^0_{\alpha\beta}(\omega) = iG^0_{\alpha}(\omega)\delta_{\alpha\beta},$$

where

$$iG^0_{\alpha}(\omega) = \frac{i}{\omega - E_\alpha + i\eta_\alpha}, \qquad \eta_\alpha = \begin{cases} +\eta, & \text{state } \alpha \text{ unoccupied} \\ -\eta, & \text{state } \alpha \text{ occupied.} \end{cases}$$

Here "occupied" and "unoccupied" refer to the occupancy of the single-particle state α in the noninteracting case.

Dyson's Equation

Dyson's equation for $iG_{\alpha\beta}$ is

$$iG_{\alpha\beta}(\omega) = iG^0_{\alpha\beta}(\omega) + iG^0_{\alpha}(\omega) \Big[-i\Sigma_{\alpha\beta}(\omega) \Big] iG_{\alpha\beta}(\omega)$$

where the self-energy $-i\Sigma_{\alpha\beta}$ is the sum of all proper self-energy diagrams, i.e. irreducible diagrams in the diagrammatic expansion of $iG_{\alpha\beta}$ with incoming and outgoing propagators excised.

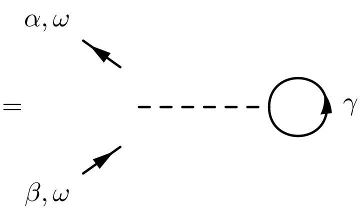
2.3 First-Order Self Energy

The first-order contributions to the self-energy are evaluated below. We note the following:

- The sum of diagrams is defined, not simply as Σ or $i\Sigma$, but $-i\Sigma$. Yes, we hate this ridiculous convention too, but it seems to be unavoidable.
- The short lines for incoming and outgoing propagators are included only as a mnemonic to get the correct placing of indices on interaction lines; the corresponding factors of iG^0 are not to be included in the evaluation of the diagrams.
- A propagator with label γ connecting two vertices of the same interaction line is evaluated as

$$iG^0_\gamma(t=0^-) = -n_\gamma = \begin{cases} -1, & \text{state } \gamma \text{ occupied} \\ 0, & \text{state } \gamma \text{ unoccupied} \end{cases}$$

$-i\Sigma^{(1a)}_{\alpha\beta}(\omega) \quad =$



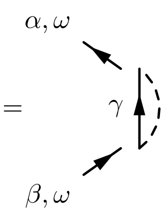
$$= (-i)^1(-1)\sum_\gamma V_{\alpha\gamma\beta\gamma}(-n_\gamma)$$

$(-i)^1$: one interaction

(-1): one fermion loop

$(-n_\gamma)$: $iG^0_\gamma(0^-)$

$-i\Sigma^{(1b)}_{\alpha\beta}(\omega) \quad =$



$$= (-i)\sum_\gamma V_{\alpha\gamma\gamma\beta}(-n_\gamma)$$

Then the full self-energy to first order is

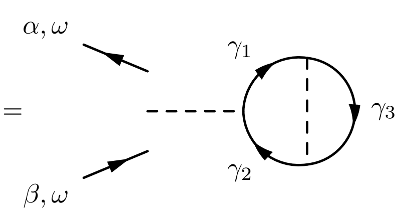
$$-i\Sigma^{(1)}_{\alpha\beta}(\omega) = -i\sum_{\gamma\text{ occupied}}\Big(V_{\alpha\gamma\beta\gamma} - V_{\alpha\gamma\gamma\beta}\Big) \qquad \text{(no frequency dependence)}$$

3 Second-Order Self Energy

The second-order contribution to the self-energy consists of six diagrams, which we label according to the convention of Fetter & Walecka Figure 9.16.

$\boxed{\sum^{2a}}$

$-i\Sigma^{(2a)}_{\alpha\beta}(\omega) \quad =$



$$= (-i)^2(-1)\sum_{\gamma_1\gamma_2\gamma_3} V_{\alpha\gamma_1\beta\gamma_2}V_{\gamma_2\gamma_3\gamma_3\gamma_1}(-n_{\gamma_3})\int\frac{d\omega'}{2\pi}iG^0_{\gamma_1}(\omega')iG^0_{\gamma_2}(\omega') \tag{1}$$

The frequency integral is

$$\int \frac{d\omega'}{2\pi} iG^0_{\gamma_1}(\omega') iG^0_{\gamma_2}(\omega') = \int \frac{d\omega'}{2\pi} \left(\frac{i}{\omega' - E_{\gamma_1} + i\eta_{\gamma_1}} \right) \left(\frac{i}{\omega' - E_{\gamma_2} + i\eta_{\gamma_2}} \right)$$
$$= \frac{-i}{2\pi i} \int d\omega' \left(\frac{1}{\omega' - E_{\gamma_1} + i\eta_{\gamma_1}} \right) \left(\frac{1}{\omega' - E_{\gamma_2} + i\eta_{\gamma_2}} \right)$$

If γ_1 and γ_2 are both occupied or both unoccupied, all the poles of the integrand lie in the same half-plane and we may close the contour in the other half-plane to conclude that the integral vanishes. If γ_1 is occupied and γ_2 is unoccupied, then (closing the integral in the upper half-plane) we pick up the pole at $\omega' = E_{\gamma_1} + i\eta$, yielding a residue of $1/(E_{\gamma_1} - E_{\gamma_2} + i\eta)$, while if γ_1 is unoccupied and γ_2 is occupied we obtain the same result with γ_1 and γ_2 reversed. Hence

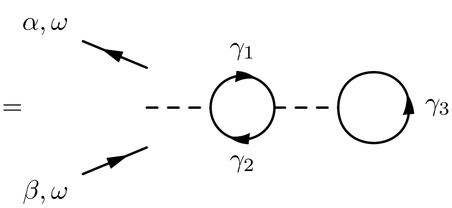
$$\int \frac{d\omega'}{2\pi} iG^0_{\gamma_1}(\omega') iG^0_{\gamma_2}(\omega') = \begin{cases} 0, & \gamma_1, \gamma_2 \text{ both occupied or both unoccupied} \\ \frac{+i}{E_{\gamma_2} - E_{\gamma_1} + i\eta}, & \gamma_1 \text{ occupied and } \gamma_2 \text{ unoccupied} \\ \frac{+i}{E_{\gamma_1} - E_{\gamma_2} + i\eta}, & \gamma_1 \text{ unoccupied and } \gamma_1 \text{ occupied} \end{cases} \tag{2}$$

Inserting into (1), we obtain

$$-i\Sigma^{(2a)}_{\alpha\beta}(\omega) = -i \sum_{\substack{\gamma_1, \gamma_3 \text{ occupied} \\ \gamma_2 \text{ empty}}} \frac{V_{\alpha\gamma_1\beta\gamma_2} V_{\gamma_2\gamma_3\gamma_3\gamma_1} + V_{\alpha\gamma_2\beta\gamma_1} V_{\gamma_1\gamma_3\gamma_3\gamma_2}}{E_{\gamma_2} - E_{\gamma_1} + i\eta} \qquad \text{(no frequency dependence)}$$

$\boxed{\Sigma^{2b}}$

$-i\Sigma^{(2b)}_{\alpha\beta}(\omega) \quad =$

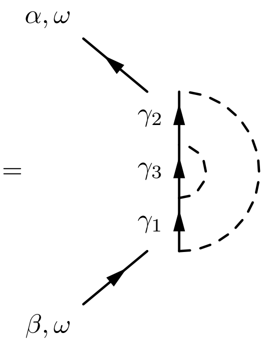


$$= (-i)^2(-1)^2 \sum_{\gamma_1\gamma_2\gamma_3} V_{\alpha\gamma_1\beta\gamma_2} V_{\gamma_2\gamma_3\gamma_1\gamma_3} (-n_{\gamma_3}) \int \frac{d\omega'}{2\pi} iG^0_{\gamma_1}(\omega') iG^0_{\gamma_2}(\omega')$$
$$= i \sum_{\substack{\gamma_1, \gamma_3 \text{ occupied} \\ \gamma_2 \text{ empty}}} \frac{V_{\alpha\gamma_1\beta\gamma_2} V_{\gamma_2\gamma_3\gamma_1\gamma_3} + V_{\alpha\gamma_2\beta\gamma_1} V_{\gamma_1\gamma_3\gamma_2\gamma_3}}{E_{\gamma_2} - E_{\gamma_1} + i\eta} \qquad \text{(no frequency dependence)} \tag{3}$$

We note that $-i\Sigma^{(2a)}$ and $-i\Sigma^{(2b)}$ are kind of like exchange (Fock) and direct (Hartree) versions of the same process.

$\boxed{\sum^{2c}}$

$-i\Sigma^{(2c)}_{\alpha\beta}(\omega) \quad =$

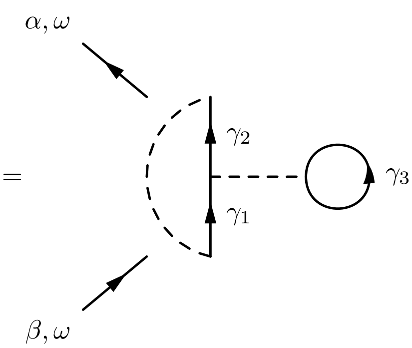


$$= (-i)^2 \sum_{\gamma_1\gamma_2\gamma_3} V_{\alpha\gamma_1\gamma_2\beta} V_{\gamma_2\gamma_3\gamma_3\gamma_1}(-n_{\gamma_3}) \int \frac{d\omega'}{2\pi} iG^0_{\gamma_1}(\omega) iG^0_{\gamma_2}(\omega)$$

$$= i \sum_{\substack{\gamma_1,\gamma_3 \text{ occupied} \\ \gamma_2 \text{ empty}}} \frac{V_{\alpha\gamma_1\gamma_2\beta}V_{\gamma_2\gamma_3\gamma_3\gamma_1} + V_{\alpha\gamma_2\gamma_1\beta}V_{\gamma_1\gamma_3\gamma_3\gamma_2}}{E_{\gamma_2} - E_{\gamma_1} + i\eta} \qquad \text{(no frequency dependence)} \tag{4}$$

$\boxed{\sum^{2d}}$

$-i\Sigma^{(2c)}_{\alpha\beta}(\omega) \quad =$



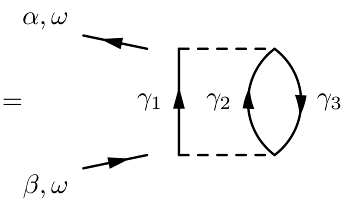
$$= (-i)^2(-1) \sum_{\gamma_1\gamma_2\gamma_3} V_{\alpha\gamma_1\gamma_2\beta} V_{\gamma_2\gamma_3\gamma_1\gamma_3}(-n_{\gamma_3}) \int \frac{d\omega'}{2\pi} iG^0_{\gamma_1}(\omega) iG^0_{\gamma_2}(\omega)$$

$$= -i \sum_{\substack{\gamma_1,\gamma_3 \text{ occupied} \\ \gamma_2 \text{ empty}}} \frac{V_{\alpha\gamma_1\gamma_2\beta}V_{\gamma_2\gamma_3\gamma_1\gamma_3} + V_{\alpha\gamma_2\gamma_1\beta}V_{\gamma_1\gamma_3\gamma_2\gamma_3}}{E_{\gamma_2} - E_{\gamma_1} + i\eta} \qquad \text{(no frequency dependence).} \tag{5}$$

We note again that $-i\Sigma^{(2c)}$ and $-i\Sigma^{(2d)}$ are like the Fock and Hartree versions of the same process.

$\boxed{\Sigma^{2e}}$

$$-i\Sigma^{(2e)}_{\alpha\beta}(\omega) \quad = $$



$$= (-i)^2(-1)\sum_{\gamma_1\gamma_2\gamma_3} V_{\alpha\gamma_3\gamma_1\gamma_2}V_{\gamma_1\gamma_2\beta\gamma_3}\int\frac{d\omega'}{2\pi}\int\frac{d\omega''}{2\pi} iG^0_{\gamma_1}(\omega')iG^0_{\gamma_2}(\omega'')iG^0_{\gamma_3}(\omega'+\omega''-\omega) \tag{6}$$

The frequency integral here is slightly more complicated. We do the ω'' integral first:

$$\int\frac{d\omega''}{2\pi} iG^0_{\gamma_2}(\omega'')iG^0_{\gamma_3}(\omega'+\omega''-\omega) = \frac{-i}{2\pi i}\int d\omega''\left(\frac{1}{\omega''-E_{\gamma_2}+i\eta_{\gamma_2}}\right)\left(\frac{1}{\omega''-(E_{\gamma_3}+\omega-\omega')+i\eta_{\gamma_3}}\right)$$

Again the result vanishes unless the poles are in different half-planes. Accounting separately for the two possibilities yields

$$\begin{aligned}
&= -i\left[\frac{n_{\gamma_2}(1-n_{\gamma_3})}{E_{\gamma_2}-(E_{\gamma_3}+\omega-\omega')+i\eta} + \frac{(1-n_{\gamma_2})n_{\gamma_3}}{(E_{\gamma_3}+\omega-\omega')-E_{\gamma_2}+i\eta}\right] \\
&= -i\left[\frac{n_{\gamma_2}(1-n_{\gamma_3})}{\omega'-(\omega+E_{\gamma_3}-E_{\gamma_2})+i\eta} - \frac{(1-n_{\gamma_2})n_{\gamma_3}}{\omega'-(\omega+E_{\gamma_3}-E_{\gamma_2})-i\eta}\right].
\end{aligned}$$

The remaining ω' integral is then

$$\frac{+i}{2\pi i}\int d\omega'\left(\frac{1}{\omega'+E_{\gamma_1}+i\eta_{\gamma_1}}\right)\left[\frac{n_{\gamma_2}(1-n_{\gamma_3})}{\omega'-(\omega+E_{\gamma_3}-E_{\gamma_2})+i\eta} - \frac{(1-n_{\gamma_2})n_{\gamma_3}}{\omega'-(\omega+E_{\gamma_3}-E_{\gamma_2})-i\eta}\right]$$

The pole of the first term in square brackets is in the lower half-plane, while the pole of the second term is in the upper half-plane. Thus if state γ_1 is occupied (pole of $iG^0_{\gamma_1}$ in upper half-plane) then only the first term in square brackets contributes, while if γ_1 is empty then only the second term contributes. The final result for the double frequency integral is

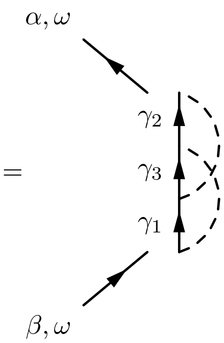
$$\begin{aligned}
&\int\frac{d\omega'}{2\pi}\int\frac{d\omega''}{2\pi} iG^0_{\gamma_1}(\omega')iG^0_{\gamma_2}(\omega'')iG^0_{\gamma_3}(\omega'+\omega''-\omega) \\
&\qquad = -i\left[\frac{n_{\gamma_1}n_{\gamma_2}(1-n_{\gamma_3})}{\omega+E_{\gamma_3}-E_{\gamma_2}-E_{\gamma_1}-i\eta} + \frac{(1-n_{\gamma_1})(1-n_{\gamma_2})n_{\gamma_3}}{\omega+E_{\gamma_3}-E_{\gamma_2}-E_{\gamma_1}+i\eta}\right]
\end{aligned} \tag{7}$$

and the final result for the self-energy is

$$-i\Sigma^{(2e)}(\omega) = -i\left[\sum_{\substack{\gamma_1,\gamma_2 \text{ occupied}\\ \gamma_3 \text{ empty}}}\frac{V_{\alpha\gamma_3\gamma_1\gamma_2}V_{\gamma_1\gamma_2\beta\gamma_3}}{\omega+E_{\gamma_3}-E_{\gamma_2}-E_{\gamma_1}-i\eta} + \sum_{\substack{\gamma_1,\gamma_2 \text{ empty}\\ \gamma_3 \text{ occupied}}}\frac{V_{\alpha\gamma_3\gamma_1\gamma_2}V_{\gamma_1\gamma_2\beta\gamma_3}}{\omega+E_{\gamma_3}-E_{\gamma_2}-E_{\gamma_1}+i\eta}\right].$$

$\boxed{\sum^{2f}}$

$$-i\Sigma^{(2f)}_{\alpha\beta}(\omega) =$$



$$= (-i)^2 \sum_{\gamma_1\gamma_2\gamma_3} V_{\alpha\gamma_3\gamma_2\gamma_1} V_{\gamma_1\gamma_2\beta\gamma_3} \int \frac{d\omega'}{2\pi} \int \frac{d\omega''}{2\pi} iG^0_{\gamma_1}(\omega') iG^0_{\gamma_2}(\omega'') iG^0_{\gamma_3}(\omega' + \omega'' - \omega)$$

$$= +i \left[\sum_{\substack{\gamma_1,\gamma_2 \text{ occupied} \\ \gamma_3 \text{ empty}}} \frac{V_{\alpha\gamma_3\gamma_2\gamma_1} V_{\gamma_1\gamma_2\beta\gamma_3}}{\omega + E_{\gamma_3} - E_{\gamma_2} - E_{\gamma_1} - i\eta} \quad + \sum_{\substack{\gamma_1,\gamma_2 \text{ empty} \\ \gamma_3 \text{ occupied}}} \frac{V_{\alpha\gamma_3\gamma_2\gamma_1} V_{\gamma_1\gamma_2\beta\gamma_3}}{\omega + E_{\gamma_3} - E_{\gamma_2} - E_{\gamma_1} + i\eta} \right]. \tag{8}$$