

GREEN FUNCTIONS

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A system of bosons or fermions is described by the Hamiltonian $H = H_1 + H_2$, where H_1 and H_2 are the one and two particle operators

$$(1) \quad H_1 = \sum_{ab} h_{ab} c_a^\dagger c_b, \quad H_2 = \frac{1}{2} \sum_{abcd} v_{abcd} c_a^\dagger c_b^\dagger c_d c_c$$

An arbitrary one-particle basis is used, with corresponding canonical operators c_a and c_a^\dagger . The matrix elements are $h_{ab} = \langle a|h|b\rangle$ and $v_{abcd} = \langle ab|v|cd\rangle = v_{badc}$ (invariance for exchange of particles).

The ground state of H is $|gs\rangle$; the Heisenberg time-evolution of an operator is $O(t) = e^{iHt/\hbar} O e^{-iHt/\hbar}$. It solves the equation of motion

$$(2) \quad i\hbar \frac{d}{dt} O(t) = e^{iHt/\hbar} [O, H] e^{-iHt/\hbar}.$$

Let us evaluate $[c_r, H]$. By means of the commutators

$$(3) \quad [c_r, c_a^\dagger c_b] = \delta_{ar} c_b$$

$$(4) \quad [c_r, c_a^\dagger c_b^\dagger c_d c_c] = (\delta_{ra} c_b^\dagger \pm \delta_{rb} c_a^\dagger) c_d c_c$$

we obtain $[c_r, H_1] = \sum_b h_{rb} c_b$ and $[c_r, H_2] = \frac{1}{2} \sum_{bcd} (v_{rbcd} \pm v_{brcd}) c_b^\dagger c_d c_c$. The indices c and d are exchanged in the second term; next the destruction operators are exchanged: $c_c c_d = \pm c_d c_c$. Then $[c_r, H_2] = \frac{1}{2} \sum_{bcd} (v_{rbcd} + v_{brdc}) c_b^\dagger c_d c_c$. Since $\langle ab|v|cd\rangle = \langle ba|v|dc\rangle$, the final expression is obtained:

$$(5) \quad \boxed{[c_r, H] = \sum_b h_{rb} c_b + \sum_{bcd} v_{rbcd} c_b^\dagger c_d c_c}$$

The following algebraic identities are useful, and simple to obtain:

Exercise 1. Show that

$$(6) \quad \sum_r c_r^\dagger [c_r, H] = H_1 + 2H_2$$

$$(7) \quad [c_r^\dagger, H] = - \sum_a c_a^\dagger h_{ar} - \sum_{abc} v_{abrc} c_a^\dagger c_b^\dagger c_c$$

$$(8) \quad i\hbar \frac{d}{dt} c_r(t) = \sum_b h_{rb} c_b(t) + \sum_{bcd} v_{rbcd} (c_b^\dagger c_d c_c)(t)$$

1. The time-ordered Green function

Let us introduce the symbol \mathbb{T} of *time-ordering of operators*. Its action on a product of creation/destruction operators of any set of states, at *different* times of Heisenberg evolution with the same Hamiltonian, is to reorder them with times decreasing from left to right:

$$(9) \quad \mathbb{T}A_1(t_1) \dots A_N(t_N) = (\pm 1)^\sigma A_{\sigma_1}(t_{\sigma_1}) \dots A_{\sigma_N}(t_{\sigma_N}), \quad t_{\sigma_1} > \dots > t_{\sigma_N}$$

σ is the permutation that produces the time-ordered product, $(\pm 1)^\sigma$ is 1 for boson statistics, or ± 1 for Fermi statistics, according to the number of exchanges in σ being even or odd.

Example: $\mathbb{T}c_r(t)c_s^\dagger(t+1)c_q(t-1) = \pm c_s^\dagger(t+1)c_r(t)c_q(t-1)$.

The definition implies that creation/destruction operators may be permuted (any permutation σ) under the symbol of \mathbb{T} -ordering, up to a sign:

$$(10) \quad \mathbb{T}A_1(t_1) \dots A_N(t_N) = (\pm 1)^\sigma \mathbb{T}A_{\sigma_1}(t_{\sigma_1}) \dots A_{\sigma_N}(t_{\sigma_N})$$

The action on a product of generic operators, in second quantization and at different times is defined by linearity.

The 1-particle time-ordered Green function is:

$$(11) \quad \boxed{iG_{rr'}(t, t') = \langle gs | \mathbb{T}c_r(t)c_{r'}^\dagger(t') | gs \rangle}$$

If the action of \mathbb{T} and the Heisenberg evolution are written explicitly, it is:

$$iG_{rr'}(t, t') = \theta(t - t') e^{-\frac{i}{\hbar} E_{gs}(t' - t)} \langle gs | c_r U(t - t') c_{r'}^\dagger | gs \rangle \\ \pm \theta(t' - t) e^{-\frac{i}{\hbar} E_{gs}(t - t')} \langle gs | c_{r'}^\dagger U(t' - t) c_r | gs \rangle$$

The interpretation is simple. If $t > t'$, the matrix element $\langle gs | c_r U(t - t') c_{r'}^\dagger | gs \rangle$ is the projection of the state $c_{r'}^\dagger | gs \rangle$, propagated in time $t - t'$, on the state $c_r^\dagger | gs \rangle$. States are not normalized: $\|c_r^\dagger | gs \rangle\|^2 = \langle gs | c_r c_r^\dagger | gs \rangle = 1 \pm n_r$. If the normalization is taken into account and if, for fermions, $n_r < 1$ and $n_{r'} < 1$,

$$|G_{r,r'}(t, t')|^2 = \frac{|\langle gs | c_r U(t - t') c_{r'}^\dagger | gs \rangle|^2}{(1 \pm n_r)(1 \pm n_{r'})} = P(r', t' \rightarrow r, t | gs)$$

is the probability that a particle created in a state r' , is observed in a state r after a time $t - t'$, indistinguishable from the particles in the ground state.

With the knowledge of the Green function, the ground-state average of any 1-particle operator may be evaluated by it:

$$(12) \quad \langle gs | c_r^\dagger c_s | gs \rangle = \langle c_r^\dagger(t^+) c_s(t) \rangle = \langle \mathbb{T} c_r^\dagger(t^+) c_s(t) \rangle = \pm i G_{sr}(t, t^+)$$

Then: $\langle O \rangle = \pm i \sum_{rs} O_{rs} G_{sr}(t, t^+)$.

2. The ground state energy

The operator identity eq.(6) yields an expression for the total energy, due to Galitskii and Migdal. First apply Heisenberg's evolution in time and use $[c_r(t), H] = i\hbar \dot{c}_r(t)$. Next take the expectation value on the exact ground state; for any operator it is $\langle gs | O(t) | gs \rangle = \langle gs | O | gs \rangle$. Then:

$$\langle gs | H_1 + 2H_2 | gs \rangle = i\hbar \sum_r \langle c_r^\dagger(t) \frac{d}{dt} c_r(t) \rangle = i\hbar \lim_{t' \rightarrow t} \sum_r \frac{\partial}{\partial t} \langle c_r^\dagger(t') c_r(t) \rangle$$

If $t' > t^+$ a T-ordering can be introduced in the inner product; this allows to exchange the operators and obtain:

$$\langle H_1 \rangle + 2\langle H_2 \rangle = \mp \hbar \lim_{t' \rightarrow t^+} \frac{\partial}{\partial t} \sum_r G_{rr}(t, t')$$

The equation provides the expectation value of the 2-particle operator H_2 in terms of the 1-particle Green function¹. The total energy is $E_{GS} = \langle H_1 \rangle + \langle H_2 \rangle$:

$$(13) \quad \boxed{E_{GS} = \pm \frac{i}{2} \lim_{t' \rightarrow t^+} \sum_{ab} \left[i\hbar \delta_{ab} \frac{\partial}{\partial t} + h_{ab} \right] G_{ba}(t, t')}$$

In the basis of position and spin, and for a potential that does not depend on spin:

$$E_{GS} = \pm \frac{i}{2} \sum_m \int d^3x \left[i\hbar \frac{\partial}{\partial t} - \frac{\hbar^2}{2m} \nabla_{\mathbf{x}}^2 + U(\mathbf{x}) \right] G_{mm}(\mathbf{x}t, \mathbf{x}'t') \Big|_{(\mathbf{x}', t')=(\mathbf{x}, t^+)}$$

Exercise 2. Show that, in presence of translation invariance and spin independent interaction, the formula simplifies to

$$\frac{E_{gs}}{V} = \pm i \frac{(2s+1)}{2} \int \frac{d^3k d\omega}{(2\pi)^4} [\hbar\omega + \epsilon(\mathbf{k})] G(\mathbf{k}, \omega) e^{i\omega\eta}$$

where V is the volume.

3. Equation of motion of the propagator

Let us evaluate

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} G_{rr'}(t, t') &= \hbar \frac{\partial}{\partial t} \left[\theta(t-t') \langle c_r(t) c_{r'}^\dagger(t') \rangle \pm \theta(t'-t) \langle c_{r'}^\dagger(t') c_r(t) \rangle \right] \\ &= \hbar \delta(t-t') \langle c_r(t) c_{r'}^\dagger(t') \mp c_{r'}^\dagger(t') c_r(t) \rangle + \hbar \langle \mathbb{T} \frac{dc_r(t)}{dt} c_{r'}^\dagger(t') \rangle \\ &= \hbar \delta(t-t') \delta_{rr'} - i \sum_b h_{rb} \langle \mathbb{T} c_b(t) c_{r'}^\dagger(t') \rangle - i \sum_{bcd} v_{rbcd} \langle \mathbb{T} (c_b^\dagger c_d c_c)(t) c_{r'}^\dagger(t') \rangle \\ \sum_b \left[\delta_{rb} i\hbar \frac{\partial}{\partial t} - h_{rb} \right] G_{br'}(t, t') &= \hbar \delta(t-t') \delta_{rr'} - i \sum_{bcd} v_{rbcd} \langle \mathbb{T} (c_b^\dagger c_d c_c)(t) c_{r'}^\dagger(t') \rangle \end{aligned}$$

In the last term, the T ordering acts on the triplet as a single operator at time t . To treat the three operators individually, the ambiguity of equal time is avoided by adding infinitesimal time shifts that keep memory of the original order:

$$\begin{aligned} \langle \mathbb{T} (c_b^\dagger c_d c_c)(t) c_{r'}^\dagger(t') \rangle &= \langle \mathbb{T} c_b^\dagger(t^{++}) c_d(t^+) c_c(t) c_{r'}^\dagger(t') \rangle \\ &= \langle \mathbb{T} c_c(t) c_d(t^+) c_{r'}^\dagger(t') c_b^\dagger(t^{++}) \rangle \end{aligned}$$

Inside a T product operators may be permuted, up to a sign. The ++ and + must be left in place as far as T is present. The matrix element has been written with creation operators at the right, to comply with the definition of the two-particle Green function:

$$(14) \quad \boxed{i^2 G_{abcd}(t_a, t_b, t_c, t_d) = \langle \mathbb{T} c_a(t_a) c_b(t_b) c_d^\dagger(t_d) c_c^\dagger(t_c) \rangle}$$

¹The single particle average is: $\langle H_1 \rangle = \mp i \sum_{ab} h_{ab} G_{ba}(t, t^+)$.

(note the positions of labels c and d). Because of \mathbb{T} -ordering:

$$(15) \quad G_{abcd}(t_a, t_b, t_c, t_d) = \pm G_{bacd}(t_b, t_a, t_c, t_d) = \pm G_{abdc}(t_a, t_b, t_d, t_c)$$

The equation of motion of the propagator is obtained:

$$(16) \quad \sum_b (i\hbar\delta_{rb}\partial_t - h_{rb})G_{br'}(t, t') = \hbar\delta_{rr'}\delta(t-t') + i \sum_{bcd} v_{rbcd}G_{cdbr'}(t, t^+, t^{++}, t')$$

It is the first equation in an infinite hierarchy, first obtained by Martin and Schwinger, where each step involves higher order Green functions.

In the position representation, for spin-independent interactions, the equation is:

$$(17) \quad (i\hbar\partial_t - h(\mathbf{x}))G_{mm'}(\mathbf{x}t, \mathbf{x}'t') = \hbar\delta_{mm'}\delta_3(\mathbf{x} - \mathbf{x}')\delta(t-t') \\ + i \sum_{m''} \int d^3y v(\mathbf{x}, \mathbf{y})G_{mm''m''m'}(\mathbf{x}t, \mathbf{y}t^+, \mathbf{y}t^{++}, \mathbf{x}'t')$$

If the particles do not interact, the equation of motion does not involve the 2-particle Green function. Let us pause for a while on Green functions of non-interacting particles.

4. Independent particles

For independent particles the Green function is a generalized function solving

$$(18) \quad (i\hbar\delta_{ab}\partial_t - h_{ab})G_{bc}^0(t, t') = \hbar\delta_{ac}\delta(t-t')$$

The equation does not have a unique solution, as one may add a solution of the homogeneous problem.

In frequency space the equation is $(\hbar\omega\delta_{ab} - h_{ab})G_{bc}^0(\omega) = \hbar\delta_{ac}$, which is recognized as the basis-projected equation for the resolvent operator:

$$(\hbar\omega - h)G^0(\omega) = \hbar$$

with $G_{ab}^0(\omega) = \langle a|G^0(\omega)|b\rangle$. The resolvent $G^0(\omega) = (\omega - h/\hbar)^{-1}$ exists for $\hbar\omega$ not in the spectrum of h and, assuming a discrete spectrum for h :

$$G_{ab}^0(\omega) = \sum_j \frac{\langle a|j\rangle\langle j|b\rangle}{\omega - \epsilon_j/\hbar}$$

To make sense of the Fourier integral for $G_{ab}^0(t, t')$ one must shift poles (and cuts) off the real axis by infinitesimal amounts. This can be done in various ways, leading to Green functions that differ by solutions of the homogeneous equation. The most useful ones are the *retarded* and the *time-ordered* Green functions.

4.1. The retarded Green function. In the retarded Green function the whole spectrum of h is slightly shifted to the lower half of the ω -plane:

$$(19) \quad G_{ab}^{0R}(\omega) =: \sum_j \frac{\langle a|j\rangle\langle j|b\rangle}{\omega - \epsilon_j/\hbar + i\eta}$$

In passing we note that the imaginary part of the diagonal matrix elements in the position basis give the *local density of states*:

$$(20) \quad -\frac{1}{\pi}\text{Im}G^{0R}(\mathbf{x}, \mathbf{x}; \omega) =: \sum_n |\langle \mathbf{x}|n\rangle|^2\delta(\omega - \omega_n)$$

The trace (which is basis-independent) is the density of states of the Hamiltonian.

Consider the inhomogeneous equation $[i\hbar\delta_{ab}\partial_t - h_{ab}]f_b(t) = g_a(t)$ with unknown $f_a(t)$ and assigned source $g_a(t)$. The general solution can be obtained with the aid of the Green function:

$$f_a(t) = f_a^0(t) + \frac{1}{\hbar} \int dt' G_{ab}^0(t, t') g_b(t');$$

where $f_a^0(t)$ solves the homogeneous equation.

Since the retarded Green function is analytic in the upper half plane, its Fourier transform to the time variables is zero for $t' > t$, by the residue theorem,

$$\begin{aligned} G_{ab}^{0R}(t, t') &= \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} G_{ab}^R(\omega) \\ &= -i\theta(t-t') \sum_n e^{-i\omega_n(t-t')} \langle a|n\rangle \langle n|b\rangle \\ &= -i\theta(t-t') \langle a|U(t, t')|b\rangle \end{aligned}$$

This feature is of great importance in physics as it expresses *causality*: the particular solution

$$f_a^R(t) = \int dt G_{ab}^{0R}(t, t') g_b(t')$$

only depends on the values $g(t')$ at $t' < t$.

In a many body system, the retarded Green function is the expectation value of the commutator (bosons) or anticommutator (fermions) at unequal times (the definition holds also for interacting systems):

$$(21) \quad \boxed{iG_{ab}^R(t, t') = \theta(t-t') \langle gs | [c_a(t), c_b^\dagger(t')]_{\mp} |gs\rangle}$$

Exercise 3. Evaluate the retarded Green function for free particles (the result does not depend on statistics)

$$\begin{aligned} iG^R(\mathbf{x}, t; \mathbf{x}', t') &= \theta(t-t') \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}') - i\omega_k(t-t')} \\ &= -\theta(t-t') \left[\frac{m}{2\pi\hbar(t-t')} \right]^{3/2} \exp \left[-i \frac{m}{2\hbar} \frac{|\mathbf{x}-\mathbf{x}'|^2}{t-t'} \right]. \end{aligned}$$

4.2. The time-ordered Green function - fermions. In the time ordered Green function the Fermi frequency divides the spectrum into a portion that gains a positive imaginary part and another that gains a negative imaginary correction:

$$(22) \quad G_{ab}^{0T}(\omega) =: \sum_n \frac{\langle a|n\rangle \langle n|b\rangle}{\omega - \omega_n + i\eta \text{sign}(\omega - \omega_F)}$$

If states are ordered according to increasing frequencies, ω_F is the highest frequency available for N fermions in the ground state.

The Fourier transform to time variables is (in position basis)

$$(23) \quad \begin{aligned} iG^{0T}(\mathbf{x}, t; \mathbf{x}', t') &= \sum_n e^{-i\omega_n(t-t')} \langle \mathbf{x}|n\rangle \langle n|\mathbf{x}'\rangle \\ &\times [\theta(t-t')\theta(\omega - \omega_F) - \theta(t'-t)\theta(\omega_F - \omega)] \end{aligned}$$

for $t > t'$ the propagation involves energy states above the Fermi frequency (particle excitations), for $t < t'$ it involves states below the Fermi frequency (hole excitations).

By means of the unperturbed (time ordered) Green function, the equation of motion for the one particle Green function can be written in integral form:

$$(24) \quad G_{mm'}(x, x') = G_{mm'}^0(x, x') + \frac{i}{\hbar} \sum_{m''m'''} \int d^4y d^4y' G_{mm'''}^0(x, y') U^0(y', y) G_{m''m''m''m'}(y', y^+, y^{++}, x')$$

The equation $G = G^0 + G^0 U^0 G_4$ can be compared with the Dyson equation for the proper self-energy, $G = G^0 + G^0 \Sigma^* G$, to express the self energy in terms of G_4 (repeated indices are summed or integrated):

$$(25) \quad \Sigma_{mm''}^*(x, y) G_{m''m'}(y, x') = \frac{i}{\hbar} U^0(x, y) G_{mm''m''m'}(x, y^+, y^{++}, x')$$

5. Hartree Fock approximation

The 2-particle Green function admits a decomposition in connected components:

$$(26) \quad G_{abcd}(t_a, t_b, t_c, t_d) = G_{ac}(t_a, t_c) G_{bd}(t_b, t_d) \pm G_{ad}(t_a, t_d) G_{bc}(t_b, t_c) + G_{abcd}^c(t_a, t_b, t_c, t_d)$$

One of the equivalent forms of Hartree Fock approximation is to neglect completely the connected part of the 2-particle Green function, meaning that the two particles evolve independently. This truncates the Martin-Schwinger hierarchy of equations at the first level. If in the equation of motion (18) for the 1-particle Green function we neglect the connected part of G_4 we obtain:

$$(27) \quad \sum_b [i\hbar\delta_{rb}\partial_t - h_{rb}] G_{br'}(t, t') = \hbar\delta_{rr'}\delta(t-t') + i \sum_{bcd} v_{rbcd} [G_{cb}(t, t^+) G_{dr'}(t, t') \pm G_{cr'}(t, t') G_{db}(t, t^+)]$$

In frequency space it is:

$$\sum_b \left(\hbar\omega\delta_{rb} - h_{rb} - \sum_{ad} v_{rabd} \langle c_a^\dagger c_d \rangle \right) G_{br'}(\omega) = \hbar\delta_{rr'} \pm \sum_{bcd} v_{rbcd} \langle c_b^\dagger c_c \rangle G_{dr'}(\omega)$$

$$G_{mm''m''m'}(\mathbf{x}t, \mathbf{y}t^+, \mathbf{y}t^{++}, \mathbf{x}'t') \approx G_{m''m'}(\mathbf{y}t, \mathbf{x}'t') G_{mm''}(\mathbf{x}t, \mathbf{y}t^+) \pm G_{m''m''}(\mathbf{y}t, \mathbf{y}t^+) G_{mm'}(\mathbf{x}t, \mathbf{x}'t')$$

Then (18) becomes a closed quadratic equation for the propagator in HF approximation:

$$\left(i\hbar \frac{d}{dt} - h(\mathbf{x}) \right) G_{mm'}^{HF}(\mathbf{x}t, \mathbf{x}'t') = \hbar\delta_{mm'}\delta_3(\mathbf{x} - \mathbf{x}')\delta(t-t') + i \sum_{m''} \int d^3y v(\mathbf{x}, \mathbf{y}) \times [G_{m''m'}^{HF}(\mathbf{y}t, \mathbf{x}'t') G_{mm''}^{HF}(\mathbf{x}t, \mathbf{y}t^+) \pm G_{m''m''}^{HF}(\mathbf{y}t, \mathbf{y}t^+) G_{mm'}^{HF}(\mathbf{x}t, \mathbf{x}'t')]$$

Since $\pm i \sum_{m''} G_{m''m''}(\mathbf{y}t, \mathbf{y}t^+) = n(\mathbf{y})$, we obtain the Hartree interaction with HF density

$$U_H(\mathbf{x}) = \int d^3y v(\mathbf{x}, \mathbf{y}) n^{HF}(\mathbf{y})$$

The equation of motion is

$$\begin{aligned} \left(i\hbar \frac{d}{dt} - h(\mathbf{x}) - U_H(\mathbf{x}) \right) G_{mm'}^{HF}(\mathbf{x}t, \mathbf{x}'t') &= \hbar \delta_{mm'} \delta_3(\mathbf{x} - \mathbf{x}') \delta(t - t') \\ &+ i \sum_{m''} \int d^3y v(\mathbf{x}, \mathbf{y}) G_{m''m'}^{HF}(\mathbf{y}t, \mathbf{x}'t') G_{mm''}(\mathbf{x}t, \mathbf{y}t^+) \end{aligned}$$

In ω space:

$$\begin{aligned} [\hbar\omega - h(\mathbf{x}) - U_H(\mathbf{x})] G_{mm'}^{HF}(\mathbf{x}, \mathbf{x}', \omega) &= \hbar \delta_{mm'} \delta_3(\mathbf{x} - \mathbf{x}') \\ &+ i \sum_{m''} \int d^3y v(\mathbf{x}, \mathbf{y}) G_{m''m'}^{HF}(\mathbf{y}, \mathbf{x}', \omega) \int \frac{d\omega'}{2\pi} G_{mm''}^{HF}(\mathbf{x}, \mathbf{y}, \omega') e^{i\eta\omega'} \end{aligned}$$

To solve the equation we assume a spectral representation typical of independent particles

$$(28) \quad \boxed{G_{mm'}^{HF}(\mathbf{x}, \mathbf{x}', \omega) = \sum_a \frac{u_a(\mathbf{x}, m) u_a(\mathbf{x}', m')^*}{\omega - \omega_a + i\eta \operatorname{sign}(\omega_a - \omega_F)}}$$

with unknown orthonormal functions u_a and real frequencies ω_a .

Insert the representation in the equation for G , multiply by $u_a(\mathbf{x}', m')$ and integrate in \mathbf{x}' and sum on m' , Because of orthogonality:

$$\begin{aligned} [\hbar\omega - h(\mathbf{x}) - U_H(\mathbf{x})] \frac{u_a(\mathbf{x}, m)}{\omega - \omega_a \pm i\eta} &= \hbar u_a(\mathbf{x}, m) \\ &+ i \sum_{m''} \int d^3y v(\mathbf{x}, \mathbf{y}) \frac{u_a(\mathbf{y}, m'')}{\omega - \omega_a \pm i\eta} \int \frac{d\omega'}{2\pi} G_{mm''}^{HF}(\mathbf{x}, \mathbf{y}, \omega') e^{i\eta\omega'} \end{aligned}$$

Here U_H is evaluated with

$$n^{HF}(\mathbf{y}) = \sum_b \sum_m |u_b(\mathbf{x}, m)|^2 \theta(\omega_F - \omega_b).$$

The integral in ω' is evaluated by residues and gives: $i \sum_b u_b(\mathbf{x}, m) u_b(\mathbf{y}, m'')^* \theta(\omega_F - \omega_b)$. Next, the limit $\omega \rightarrow \omega_a$ is taken, and the system of Hartree-Fock equations is obtained:

$$(29) \quad \begin{aligned} [h(\mathbf{x}) + U_H(\mathbf{x})] u_a(\mathbf{x}, m) - \sum_{b, m''} \theta(\omega_F - \omega_b) u_b(\mathbf{x}, m) \\ \times \int d^3y v(\mathbf{x}, \mathbf{y}) u_a(\mathbf{y}, m'') u_b(\mathbf{y}, m'')^* = \hbar \omega_a u_a(\mathbf{x}, m) \end{aligned}$$

The spin dependence may be chosen to factorize (then it is a quantum number): $u_{a,\sigma}(\mathbf{x}, m) = f_{a\sigma}(\mathbf{x}) v_\sigma(m)$. Then: $\sum_{m''} v_\sigma(m'') v_{\sigma'}(m'') = \delta_{\sigma\sigma'}$ and

$$\begin{aligned} [h(\mathbf{x}) + U_H(\mathbf{x})] f_{a\sigma}(\mathbf{x}) - \sum_b \theta(\omega_F - \omega_b) f_{b\sigma}(\mathbf{x}) \int d^3y v(\mathbf{x}, \mathbf{y}) f_{a\sigma}(\mathbf{y}) f_{b\sigma}(\mathbf{y})^* \\ = \hbar \omega_a f_{a\sigma}(\mathbf{x}) \end{aligned}$$

If the Hartree Fock approximation is done in eq.(26), one reads the HF approximation for the self energy:

$$(30) \quad \begin{aligned} \Sigma_{mm'}^*(x, x') &= \frac{i}{\hbar} G_{mm'}^{HF}(x, x'^+) U^0(x, x') \\ &\pm \frac{i}{\hbar} \delta_{mm'} \delta_4(x - x') \sum_{m''} \int d^4y U^0(x, y) G_{m''m''}^{HF}(y, y^+) \end{aligned}$$

Therefore, we obtained another characterization of the Hartree Fock approximation: the HF self-energy is provided by the two self energy graphs of first order expansion, with the self-consistent G^{HF} replacing G^0 .

An important remark is that the Hartree-Fock self-energy is independent of time.

Exercise 4. Evaluate the HF self-energy (31), by using the expansion (29) with functions that factorize.

Exercise 5. Show that the HF self-energy $\Sigma^*(k)$ for fermions with only two-body interaction $v(|\mathbf{x} - \mathbf{y}|)$ coincides with the correction to the energy of a free fermion.

Exercise 6. Show that the self energy may be viewed as a bilocal potential in HF equations:

$$\left(i\hbar \frac{d}{dt} - h(\mathbf{x}) \right) u_a(\mathbf{x}m) - \hbar \sum_{m'} \int d^3y \Sigma_{mm'}^*(\mathbf{x}, \mathbf{x}') u_a(\mathbf{x}'m') = \hbar \omega_a u_a(\mathbf{x}m)$$