EQUATIONS OF MOTION

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1. Equation of motion of destruction operators

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

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

An arbitrary one-particle basis is used, with correspondent canonical operators c_a and $c_a^\dagger$. The matrix elements are $h_{ab} = \langle a|h|b\rangle$ and $v_{abcd} = \langle ab|v|cd\rangle = v_{badc}$ (exchange symmetry).
The time evolution of a destruction operator, $c_r(t) = e^{iHt/\hbar} c_r e^{-iHt/\hbar}$, solves the equation of motion $i\hbar\frac{d}{dt}c_r(t) = e^{iHt/\hbar}[c_r, H]e^{-iHt/\hbar}$. By means of the commutators

$$[c_r, c_a^\dagger c_b] = \delta_{ar} c_b \tag{2}$$

$$[c_r, c_a^\dagger c_b^\dagger c_d c_c] = (\delta_{ra} c_b^\dagger \pm \delta_{rb} c_a^\dagger) c_d c_c \tag{3}$$

one evaluates $[c_r, H_1] = \sum_b h_{rb} c_b$ and $[c_r, H_2] = \frac{1}{2}\sum_{bcd}(v_{rbcd} \pm v_{brcd}) c_b^\dagger c_d c_c$. First the dummy 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 $[\psi_r, H_2] = \frac{1}{2}\sum_{bcd}(v_{rbcd} + v_{brdc}) c_b^\dagger c_d c_c$. Because of the exchange symmetry the two matrix elements are equal, and the final expression is obtained:

$$\boxed{[c_r, H] = \sum_b h_{rb} c_b + \sum_{bcd} v_{rbcd} c_b^\dagger c_d c_c} \tag{4}$$

An immediate consequence is the useful operator identity:

$$\sum_r c_r^\dagger [c_r, H] = H_1 + 2H_2 \tag{5}$$

Another consequence is the equation of motion of a destruction operator:

$$i\hbar\frac{d}{dt}c_r(t) = \sum_b h_{rb} c_b(t) + \sum_{bcd} v_{rbcd}(c_b^\dagger c_d c_c)(t) \tag{6}$$

Exercise 1. *Obtain the equation of motion of the creation operator.*

Exercise 2. *Evaluate $[c_r^\dagger c_s, H]$ (it is the starting point for the "Time-dependent Hartree-Fock approximation").*

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2. The ground state energy

Eq.(5) yields an expression for the total energy, due to Galitskii and Migdal. The expectation value on the exact ground state is

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

Since $t' > t$ a T-ordering can be introduced in the inner product. This allows to exchange the operators and obtain:

$$\langle H_1 + 2H_2\rangle = \mp\hbar\frac{d}{dt}\sum_r G_{rr}(t,t^+) \tag{7}$$

where the one-particle Green function, in a generic basis, is:

$$\begin{aligned} iG_{rr'}(t,t') &= \langle \mathrm{T} c_r(t)c_{r'}^\dagger(t')\rangle \\ &= \theta(t-t')\langle c_r(t)c_{r'}^\dagger(t')\rangle \pm \theta(t'-t)\langle c_{r'}^\dagger(t')c_r(t)\rangle \end{aligned} \tag{8}$$

The equation provides the expectation value of the interaction in terms of the one-particle Green function[1]. The total energy is $E_{gs} = \langle H_1\rangle + \langle H_2\rangle$:

$$\boxed{E_{gs} = \pm\frac{i}{2}\lim_{t'\to t^+}\sum_{ab}\left[i\hbar\delta_{ab}\frac{\partial}{\partial t} + h_{ab}\right]G_{ba}(t,t')} \tag{9}$$

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

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

Exercise 3. *Show that, in presence of space-time translation invariance and spin independent interaction, the formula* (9) *simplifies to*

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

where V is the volume. Evaluate the integrals for the ideal electron gas.

3. Equation of motion of the propagator

Let us evaluate

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

In the last term, the T ordering acts on the triplet as a single operator. To treat the three operators individually, the ambiguity of equal time is avoided by adding

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

infinitesimal time shifts that keep memory of the original order:

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

The T product allows to permute operators freely, 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:

$$\boxed{i^2 G_{abcd}(t_a,t_b,t_c,t_d) = \langle T c_a(t_a) c_b(t_b) c_d^\dagger(t_d) c_c^\dagger(t_c)\rangle} \tag{10}$$

(note the positions of labels c and d). Because of $T-$ordering:

$$G_{abcd}(t_a,t_b,t_c,t_d) = \pm\, G_{bacd}(t_b,t_a,t_c,t_d) = \pm\, G_{abdc}(t_a,t_b,t_d,t_c) \tag{11}$$

The equation of motion of the propagator is obtained:

$$\begin{aligned}\sum_b \left(i\hbar\frac{\partial}{\partial t}\delta_{rb} - h_{rb}\right) G_{br'}(t,t') = \hbar\delta_{rr'}\delta(t-t') \\ + i\sum_{bcd} v_{rbcd} G_{cdbr'}(t,t^+,t^{++},t')\end{aligned} \tag{12}$$

It is the first of an infinite hierarchy of equations, first obtained by Martin and Schwinger, which involve higher order Green functions at each step.
In position representation, for spin independent interactions, the equation (12) is:

$$\begin{aligned}\left(i\hbar\frac{\partial}{\partial t} - h(\vec{x})\right) G_{mm'}(\vec{x}t,\vec{x}'t') = \hbar\delta_{mm'}\delta_3(\vec{x}-\vec{x}')\delta(t-t') \\ + i\sum_{m''}\int d^3y\; v(\vec{x},\vec{y})\, G_{mm''m''m'}(\vec{x}t,\vec{y}t^+,\vec{y}t^{++},\vec{x}'t')\end{aligned} \tag{13}$$

In 4-dimensional notation, with $U^0(x,x') =: v(\vec{x},\vec{x}')\delta(t-t')$:

$$\begin{aligned}\left(i\hbar\frac{\partial}{\partial t} - h(\vec{x})\right) G_{mm'}(x,x') = \hbar\delta_{mm'}\delta_4(x-x') \\ + i\sum_{m''}\int d^4y\, U^0(x,y) G_{mm''m''m'}(x,y^+,y^{++},x')\end{aligned} \tag{14}$$

If the two-particle interaction is absent, the equation of motion does not involve higher order functions. 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 that solves the equation

$$[i\hbar\delta_{ab}\partial_t - h_{ab}] G^0_{bc}(t,t') = \hbar\delta_{ac}\delta(t-t') \tag{15}$$

Its very usefulness appears in the solution of 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 is the sum of the general solution of the homogeneus equation $f^0_a(t)$ and a particular solution. The latter can be generated through the Green function:

$$f_a(t) = f^0_a(t) + \frac{1}{\hbar}\int dt' G^0_{ab}(t,t')g_b(t').$$

It must be noted that (15) does not have a unique solution (we have the freedom to add a solution of the homogeneous problem). This is better seen in frequency space, where (15) is: $[\hbar\omega\delta_{ab} - h_{ab}]G^0_{bc}(\omega) = \hbar\delta_{ac},$. which is the basis-projected equation for the resolvent operator:

$$[\hbar\omega\mathbb{I} - h]\; G^0(\omega) = \hbar\,\mathbb{I}$$

with $G^0_{ab}(\omega) = \langle a|G^0(\omega)|b\rangle$. The solution is well defined for $\omega \in \mathbb{C}/\sigma(h)$.
The Fourier integral of $G^0_{ab}(\omega)$ back to $G^0_{ab}(t,t')$ runs on the real axis. The poles and cuts (i.e. the real spectrum of the single particle Hamiltonian h) has to be shifted off the real axis by an infinitesimal amount. This can be done in various ways, that lead 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 shifted by an infinitesimal amount into the lower half-plane of the $\omega-$plane:

$$G^{0R}_{ab}(\omega) =: \langle a|(\omega - h/\hbar + i\eta)^{-1}|b\rangle = \sum_n \frac{\langle a|n\rangle\langle n|b\rangle}{\omega - \omega_n + i\eta} \tag{16}$$

where $h|n\rangle = \hbar\omega_n|n\rangle$, and we neglect the continuum. In passing we note that the imaginary part of the diagonal matrix elements in the position basis give the *local density of states*:

$$-\frac{1}{\pi}\mathrm{Im}\, G^{0R}(\vec{x},\vec{x};\omega) =: \sum_n |\langle\vec{x}|n\rangle|^2\delta(\omega-\omega_n) \tag{17}$$

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

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

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

$$f^R_a(t) = \int dt\, G^{0R}_{ab}(t,t')\, g_b(t')$$

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):

$$\boxed{iG^R_{ab}(t,t') = \theta(t-t')\,\langle gs|\left[c_a(t), c_b^\dagger(t')\right]_\mp |gs\rangle} \tag{18}$$

Exercise 4. *Evaluate the retarded Green function for free particles (the result does not depend on statistics)*

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

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

$$G^{0T}_{ab}(\omega) =: \sum_n \frac{\langle a|n\rangle\langle n|b\rangle}{\omega-\omega_n+i\eta\,\mathrm{sign}(\omega-\omega_F)} \tag{19}$$

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)

$$\begin{aligned} iG^{0T}(\vec{x},t;\vec{x}',t') = &\sum_n e^{-i\omega_n(t-t')}\langle\vec{x}|n\rangle\langle n|\vec{x}'\rangle \\ &\times\left[\theta(t-t')\theta(\omega-\omega_F)-\theta(t'-t)\theta(\omega_F-\omega)\right] \end{aligned} \tag{20}$$

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:

$$\begin{aligned} G_{mm'}(x,x') = G^0_{mm'}(x,x') + \frac{i}{\hbar}\sum_{m''m'''}\int d^4y\,d^4y' \\ G^0_{mm'''}(x,y')U^0(y',y)G_{m'''m''m''m'}(y',y^+,y^{++},x') \end{aligned} \tag{21}$$

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

$$\Sigma^\star_{mm''}(x,y)G_{m''m'}(y,x') = \frac{i}{\hbar}U^0(x,y)G_{mm''m''m'}(x,y^+,y^{++},x') \tag{22}$$

5. Hartree Fock approximation

The two-particle Green function admits a decomposition into connected components:

$$\begin{aligned} &G_{abcd}(t_a,t_b,t_c,t_d) \\ &= G_{ac}(t_a,t_c)G_{bd}(t_b,t_d) \pm G_{ad}(t_a,t_d)G_{bc}(t_b,t_c) + G^c_{abcd}(t_a,t_b,t_c,t_d) \end{aligned} \tag{23}$$

One of the several equivalent ways to perform the Hartree Fock approximation is to neglect completely the connected part of the two particle Green function, meaning that the two particles evolve independently. This truncates the Martin-Schwinger hierarchy of equations at the first level. In the equation of motion (13) for the one particle Green function we approximate:

$$\begin{aligned}&G_{mm''m''m'}(\vec{x}t,\vec{y}t^+,\vec{y}t^{++},\vec{x}'t')\\&\approx G_{m''m'}(\vec{y}t,\vec{x}'t')G_{mm''}(\vec{x}t,\vec{y}t^+)\pm G_{m''m''}(\vec{y}t,\vec{y}t^+)G_{mm'}(\vec{x}t,\vec{x}'t')\end{aligned}$$

Then (13) becomes a closed quadratic equation for the propagator in HF approximation:

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

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

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

The equation of motion is

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

In ω space:

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

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

$$\boxed{G^{HF}_{mm'}(\vec{x},\vec{x}',\omega)=\sum_a\frac{u_a(\vec{x},m)u_a(\vec{x}',m')^*}{\omega-\omega_a+i\eta\,\mathrm{sign}\,(\omega_a-\omega_F)}}\tag{24}$$

with unknown orthonormal functions u_a and real frequencies ω_a.
Insert the representation in the equation for G, multiply by $u_a(\vec{x}',m')$ and integrate in $\vec{x}'$ and sum on m', Because of orthogonality:

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

Here U_H is evaluated with

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

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

$$[h(\vec{x})+U_H(\vec{x})]\,u_a(\vec{x},m)-\sum_{b,m''}\theta(\omega_F-\omega_b)u_b(\vec{x},m) \times\int d^3y\; v(\vec{x},\vec{y})\; u_a(\vec{y},m'')u_b(\vec{y},m'')^*=\hbar\omega_a u_a(\vec{x},m) \tag{25}$$

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

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

If the Hartree Fock approximation is done in eq.(22), one reads the HF approximation for the self energy:

$$\begin{aligned}\Sigma^\star_{mm'}(x,x')=&\frac{i}{\hbar}G^{HF}_{mm'}(x,x'^+)U^0(x,x')\\ &\pm\frac{i}{\hbar}\delta_{mm'}\delta_4(x-x')\sum_{m''}\int d^4y\,U^0(x,y)G^{HF}_{m''m''}(y,y^+)\end{aligned} \tag{26}$$

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 5. *Evaluate the HF self-energy* (26)*, by using the expansion* (24) *with functions that factorize.*

Exercise 6. *Show that the HF self-energy $\Sigma^\star(k)$ for fermions with only two-body interaction $v(|\vec{x}-\vec{y}|)$ coincides with the correction to the energy of a free fermion.*

Exercise 7. *Show that the self energy may be viewed as a bilocal potential in HF equations:*

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