1.3 The general form of the Green's function in frequency space

1.3.1 The free Green's function (fermions)

We consider a system of free fermions with the Hamiltonian

$$H = \sum_{p\sigma} \varepsilon_p \, c^+_{p\sigma} c_{p\sigma}$$

From the equation of motion of the operators,

$$i \frac{d}{dt} c_{p\sigma} = \left[c_{p\sigma}, H - \mu \right] = (\varepsilon_p - \mu)\, c_{p\sigma} \, ,$$

one obtains the equation of motion (EOM) of the Green's function,

$$G_{p\sigma}(t) = -i \left\langle\!\left\langle T \left\{ c_{p\sigma}(t)\, c^+_{p\sigma}(0) \right\} \right\rangle\!\right\rangle$$

$$\text{with } \langle\!\langle \ldots \rangle\!\rangle = tr \left\{ \frac{e^{-\beta(H-\mu N)}}{Z_G} \ldots \right\}$$

(which is diagonal in $\vec{p}, \sigma$ for a translation and spin rotation invariant system)

as

$$\boxed{\left(i \frac{d}{dt} + \mu - \varepsilon_p \right) G_{p\sigma}(t) = \delta(t).}$$

The "$\delta(t)$" arises from the differentiation of the $\theta(\pm t)$ functions involved in the time ordering.

Note that the EOM is the same for G, G^R, G^R.
Only the different boundary conditions in time distinguish the three types of solutions.

By Fourier transformation one obtains at $T=0$

$$G_{p\sigma}(\omega) = \frac{1}{\omega+\mu-\varepsilon_p+i\eta\,\mathrm{sgn}(\varepsilon_p-\mu)}$$

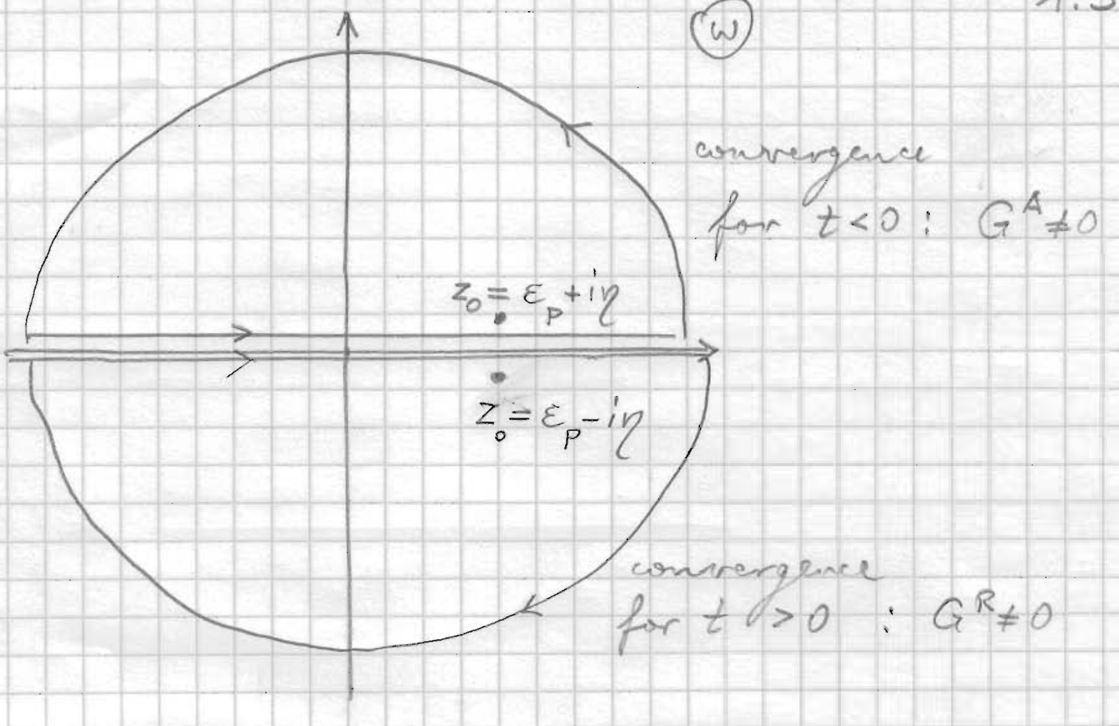
This is in agreement with the spectral representation, where for the non-interacting system the spectral function is $A(\vec{p},\omega) = \delta(\omega+\mu-\varepsilon_p)$.

The free retarded G-functions are (for any T)

$$G^{R/A}_{p\sigma}(\omega) = \frac{1}{\omega+\mu-\varepsilon_p \pm i\eta},$$

again in agreement with the spectral representation.

The fact that $G^{R/A}(t) \neq 0$ for $t \gtrless 0$ requires via contour integration that in the ω-domain $G^R(\omega)$ / $G^A(\omega)$ has a pole in the <u>lower</u>/<u>upper</u> ω half plane, respectively.
This is obeyed by the above expression for $G^{R/A}$ and is in accordance with the analyticity of $G^{R/A}(\omega)$ in the <u>upper</u> / <u>lower</u> half plane.



$$G^{R/A}(t) = \int \frac{d\omega}{2\pi}\, e^{-i\omega t}\, G^{R/A}(\omega)$$

1.3.2 The physical meaning of the pole

We will see by explicit calculation ($\to$ perturbation theory) that due to interactions the pole of $G^{R/A}(\omega)$ at $\omega = z_0$ is shifted away from the real axis, i.e. z_0 acquires a finite imaginary part, given by the selfenergy $\Sigma^{R/A}_{p\sigma}(\omega)$ which is in general a function of $\vec{p}$ and ω and in a magnetic system also of σ.
In an interacting system the R/A Green's function hence takes the form

$$\boxed{G^{R/A}_{\vec{p}\sigma}(\omega) = \frac{1}{\omega + \mu - \varepsilon_p - \Sigma^{R/A}_{p\sigma}(\omega)}}$$

with $\mathrm{Im}\,\Sigma^{R/A} \lessgtr 0$

To understand the physical meaning of the pole we transform to time space (contour integration) using the position and the residue of the pole.

<u>position</u>: $\omega + \mu - \varepsilon_p - \Sigma^{R/A}_{\vec{p}\sigma}(\omega) = 0$

Expanding this for not too large $\mathrm{Re}\,\Sigma_p(\omega)$ about the non-interacting pole position,

$$\Sigma^{R/A}_{p\sigma}(\omega) = \Sigma^{R/A}_{p\sigma}(\varepsilon_p - \mu) + \left.\frac{d\Sigma^{R/A}_{p\sigma}}{d\omega}\right|_{\omega = \varepsilon_p - \mu \equiv \omega_0} (\omega + \mu - \varepsilon_p) + O\left[(\omega + \mu - \varepsilon_p)^2\right]$$

we have in the vicinity of the pole

$$G^{R/A}_{p\sigma}(\omega) = \frac{\left(1 - \left.\frac{d\Sigma^{R/A}_{p\sigma}}{d\omega}\right|_{\omega_0}\right)^{-1}}{\omega + \mu - \varepsilon_p - \frac{\Sigma^{R/A}_{p\sigma}(\varepsilon_p - \mu)}{1 - \left.\frac{d\Sigma^{R/A}}{d\omega}\right|_{\omega_0}}}$$

+ incoherent contributions.

$$G^{R/A}_{p\sigma}(\omega) = \frac{Z_{p\sigma}}{\omega + \mu - \tilde{\varepsilon}_p + i\gamma^{R/A}_p} + \text{incoherent contributions} \qquad (*)$$

$$Z_{p\sigma} = \left(1 - \left.\frac{d\Sigma^{R/A}_{p\sigma}}{d\omega}\right|_{\omega = \varepsilon_p - \mu}\right)^{-1}$$ quasiparticle weight

$$\tilde{\varepsilon}_{p\sigma} = \varepsilon_p + \mathrm{Re}\left(Z_p\, \Sigma^{R/A}_{p\sigma}(\varepsilon_p - \mu)\right)$$ renormalized q.p. dispersion

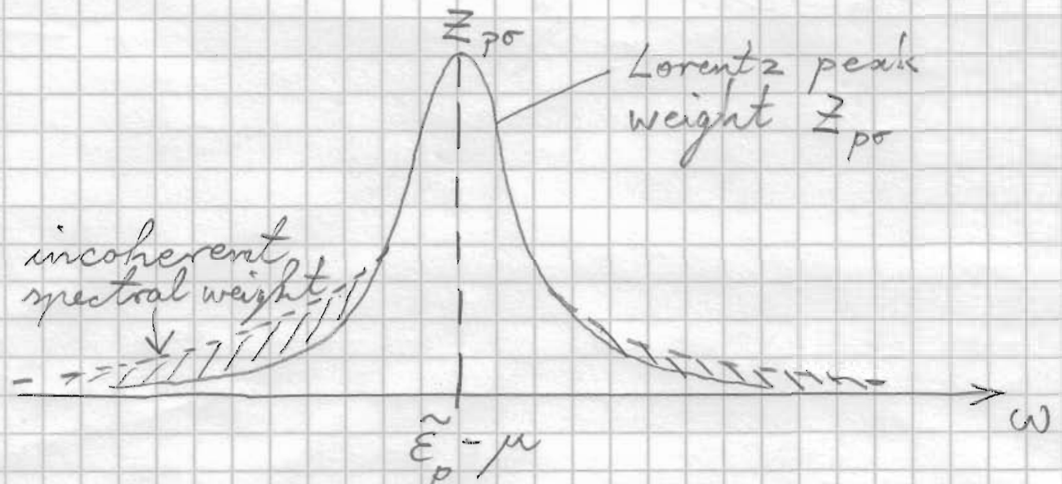
$$\gamma^{R/A}_{p\sigma} = -\mathrm{Im}\left(Z_p\, \Sigma^{R/A}_{p\sigma}(\varepsilon_p - \mu)\right) \gtrless 0$$ q.p decay rate

The physical meaning of $Z_p, \tilde{\varepsilon}_p, \gamma_{p\sigma}$ follows directly from the Fourier transformation:

$$G^R_{p\sigma}(t) = -i\ \Theta(t)\ Z^R_{p\sigma}\ e^{-i\tilde{\varepsilon}_{p\sigma} t - \gamma^R_{p\sigma} t}$$

$$+ \text{ incoherent terms}$$

<u>spectral function:</u> $\quad A_\sigma(\hat{p}, \omega) = -\frac{1}{\pi} \operatorname{Im} G^R_{p\sigma}(\omega)$



The q.p. weight $Z_{p\sigma}$ gives the fraction of coherent q.p. propagation in the G-function.
The rest of the spectral weight does not describe propagation of a single "coherent" particle but is due to many-particle excitations.

1.4 Many-body perturbation theory

1.4.1 Interaction representation of the G-function

We separate the Hamiltonian into a non-interacting part H_0, whose dynamics are known, and a perturbation V

$$H = H_0 + V$$

To develop a perturbation expansion of the exponentials in G in terms of V it is convenient to separate the time evolution wrt. H_0 from the total time evolution:

$$e^{-i(H-\mu N)t} =: e^{-i(H_0-\mu N)t} S(t)$$

and define the state in the interaction representation

$$|\Psi(t)\rangle_I = S(t)\,|\Psi(0)\rangle$$

where the time evolution in interaction representation is

$$S(t) = e^{+i(H_0-\mu N)t}\, e^{-i(H-\mu N)t}$$

It has the equation of motion

$$i\frac{d}{dt}S(t) = V_I(t)\,S(t) \qquad (*)$$

and all field operators evolve wrt. the free Hamiltonian

$$c_I(t) = e^{+i(H_0-\mu N)t} \, c \, e^{-i(H_0-\mu N)t}$$

$$V_I(t) = e^{+i(H_0-\mu N)t} \, V \, e^{-i(H_0-\mu N)t}$$

By formally integrating the equation of motion (*) for $S(t)$ (→ Lippmann-Schwinger Eq.) and iterating it, one obtains, analogous to single-particle time-dependent perturb. theory

$$S(t) = \hat{T} \, e^{-i\int_{-\infty}^{t} dt' V(t')} .$$

On the imaginary time axis one has, $\underline{t \to -i\tau}$

$$\boxed{S(\tau) = \hat{T} \, e^{-\int_0^{\tau} d\tau' V(\tau')}} \qquad 0 \le \tau \le \beta$$

with $\hat{T}$ the τ-ordering operator along the imaginary axis.

From now on we use the imaginary time representation. The continuation to $G^{R/A}$ is straight-forward in ω-space, see section 1.2.3.

Definition: $$S(\tau_2,\tau_1) := \hat{T} e^{-\int_{\tau_1}^{\tau_2} d\tau' V(\tau')}$$
$$0 \le \tau_1, \tau_2 \le \beta$$

$S(\tau_2,\tau_1)$ obeys the important multiplication rule

$$\boxed{S(\tau_2,\tau_1) = \hat{T}\left[S(\tau_2,\tau_3)\, S(\tau_3,\tau_1)\right]}$$

Proof:

$$\hat{T}\left[S(\tau_2,\tau_3)\, S(\tau_3,\tau_1)\right] = \hat{T}\left[\left(\hat{T} e^{-\int_{\tau_3}^{\tau_2} d\tau' V_I(\tau')}\right)\left(\hat{T} e^{-\int_{\tau_1}^{\tau_3} d\tau'' V_I(\tau'')}\right)\right]$$
$$= \hat{T}\left[e^{-\int_{\tau_3}^{\tau_2} d\tau' V_I(\tau') - \int_{\tau_1}^{\tau_3} d\tau'' V_I(\tau'')}\right] = S(\tau_2,\tau_1) \quad \blacksquare$$

In particular:

$$S(\tau_2,\tau_1) = \hat{T}\left[S(\tau_2)\, S^{-1}(\tau_1)\right]$$

The thermal Green's function is expressed in the interaction representation as

$$G(\vec{r},\vec{r}\,',\tau) = -\frac{tr\left\{\hat{T}\left[e^{-(H-\mu N)\beta} e^{(H-\mu N)\tau} \psi(\vec{r}) e^{-(H-\mu N)\tau} \psi^{+}(\vec{r}\,')\right]\right\}}{tr\left\{e^{-(H-\mu N)\beta}\right\}}$$

$$= -\frac{tr\left\{\hat{T}\left[e^{-(H_0-\mu N)\beta} S(\beta)\, S^{-1}(\tau) e^{(H_0-\mu N)\tau} \psi(\vec{r}) e^{-(H_0-\mu N)\tau} S(\tau) \psi^{+}(\vec{r}\,')\right]\right\}}{tr\left\{e^{-(H_0-\mu N)\beta} S(\beta)\right\}}$$

$$= -\frac{tr\left\{e^{-(H_0-\mu N)\beta}\, \hat{T}\left[\psi_I(\vec{r},\tau)\, \psi_I^{+}(\vec{r}\,',0)\, S(\beta)\right]\right\}}{tr\left\{e^{-(H_0-\mu N)\beta} S(\beta)\right\}}$$

for $0 \le \tau \le \beta$

In this expression $\hat{T}$ places each term of $S(\beta)$ in the correct place between $\psi(\tau)$, $\psi^+(0)$, and the multiplication rule for $S(\tau_2, \tau_1)$ has been used.

The perturbation theory is now developed as an expansion in powers of V_I. This requires to evaluate expectation values of higher-order products of field operators with equal numbers of ψ and of ψ^+.
This is substantially facilitated by a factorization rule, Wick's theorem.

1.4.2 Wick's theorem

We define the <u>many-particle Green's function</u> for a non-interacting system as

$$G_n^0(\tau_1, \dots, \tau_n; \tau_1', \dots, \tau_n') =$$
$$= -\frac{1}{Z_G^0} \, tr\left\{ e^{-(H_0 - \mu N)\beta} \hat{T}\left\{ \psi(\tau_1) \dots \psi(\tau_n) \psi^+(\tau_1') \dots \psi^+(\tau_n') \right\}\right\}$$

where all operators are in the interaction picture:

$$\psi(\tau_i) = e^{(H_0 - \mu N)\tau_i} \psi \, e^{-(H_0 - \mu N)\tau_i} \quad \text{etc.}$$

The factorization of the tr of operator products is derived using the equation of motion for G:

The EOM for the thermal single-particle Green's fct. is

$$\left[-\frac{\partial}{\partial t} - (H_0-\mu N)_{\tau}\right] G(\tau,\tau') = \delta(\tau-\tau')$$

acting on the operator at time τ

The EOM for the non-interacting n-particle Green's function is then obtained as

$$\left[-\frac{\partial}{\partial \tau_i} - (H_0-\mu N)_{\tau_i}\right] G_n^0(\tau_1,\dots,\tau_n;\tau_1',\dots,\tau_n')$$

$$= \sum_{j=1}^{n} (\overset{F}{\underset{B}{\mp}} 1)^{j-1+n-i}\, \delta(\tau_i-\tau_j')\, G_{n-1}^0(\tau_1,\dots,\cancel{\tau_i},\dots\tau_n;\tau_1',\dots,\cancel{\tau_j'},\dots,\tau_n')$$

number of commutations needed to bring $\psi^+(\tau_j')$ and $\psi(\tau_i)$ together.

$${}^{s}G_n^0(\tau_1,\dots,\tau_n,\tau_1',\dots\tau_n') \underset{\text{s.p. EOM}}{=} \sum_{j=1}^{n} (\mp 1)^{j-1+n-i}\, G(\tau_i,\tau_j')\, G_{n-1}^0(\tau_1\dots\cancel{\tau_i}\dots\tau_n;\tau_1'\dots\cancel{\tau_j'}\dots\tau_n')$$

By induction it follows <u>Wick's theorem</u>:

> The non-interacting n-particle Green's function (of operators with canonical commutation relations!) factorizes into a sum over products of free 1-particle Green's functions $G_1^0(\tau_i,\tau_j')$
> The sum runs over all possible pairings of operators $\psi(\tau_i)$, $\psi^+(\tau_j')$
> For each pair there is a factor $(\mp 1)^P$ (fermions/bosons) where P is the number of elementary commutations required to bring the respective operators together.

1,4,3 Feynman diagrams

Using the interaction operator in interaction repr.,

$$V(\tau) = \int d^3r_1 \int d^3r_2 \; \Psi^+(\vec{r}_1,\tau)\,\Psi^+(\vec{r}_2,\tau)\,V(\vec{r}_1-\vec{r}_2)\,\Psi(\vec{r}_2,\tau)\,\Psi(\vec{r}_1,\tau)$$

one obtains for the Green's function by expanding $S(\beta)$ in powers of V (where $x := (\vec{r},\tau)$, and x may also include a spin or other internal degree of freedom),

$$G(x,x') = -\,\frac{tr\{e^{-(H_0-\mu N)\beta}\,\hat{T}[\Psi(x)\,\Psi^+(x')\,S(\beta)]\}}{tr\{e^{-(H_0-\mu N)\beta}\,S(\beta)\}}$$

$$= \frac{1}{(Z_G/Z_{G0})}\Big[-\langle \hat{T}[\Psi(x)\,\Psi^+(x')]\rangle_0 \;+$$

$$-(-1)\int d^4x_1 \int d^4x_2 \; V(x_1-x_2)\,\langle \hat{T}[\Psi(x)\,\Psi^+(x')\;\Psi^+(x_1)\,\Psi^+(x_2)\,\Psi(x_2)\,\Psi(x_1)]\rangle_0$$

$$-(-1)^2\frac{1}{2!}\int d^4x_1 \int d^4x_2 \int d^4x_3 \int d^4x_4 \; V(x_1-x_2)\,V(x_3-x_4)\,\cdot$$

$$\langle \hat{T}[\Psi(x)\,\Psi^+(x')\;\Psi^+(x_1)\,\Psi^+(x_2)\,\Psi(x_2)\,\Psi(x_1)\,\Psi^+(x_3)\,\Psi^+(x_4)\,\Psi(x_4)\,\Psi(x_3)]\rangle_0$$

$$+\; O(V^3)\;\Big]$$

with $Z_G^0 = tr\{e^{-(H_0-\mu N)\beta}\}$ grand canonical partition function of the non-interacting system

$\langle \ldots \rangle_0 = \frac{1}{Z_G^0} tr\{e^{-(H_0-\mu N)\beta} \ldots\}$ thermal avg. for non-interacting system

$\int d^4x_1 \ldots = \int_0^\beta d\tau_1 \int d^3r_1 \ldots \qquad x_1 = (\vec{r}_1, \tau_1)$ etc.

$V(x_1 - x_2) = V(\vec{r}_1 - \vec{r}_2)\,\delta(\tau_1 - \tau_2)$
instantaneous interaction

Using Wick's theorem, the terms of $G(x,x')$ can be factorized as follows

$$G(x,x') = \frac{1}{Z_G/Z_G^0}\Big[G_0(x,x') +$$

$$+ (-1)(\mp 1) \int d^4x_1 \int d^4x_2\, G_0(x,x_2) G_0(x_2,x') V(x_1-x_2) G_0(x_1,x_1) \qquad (A)$$

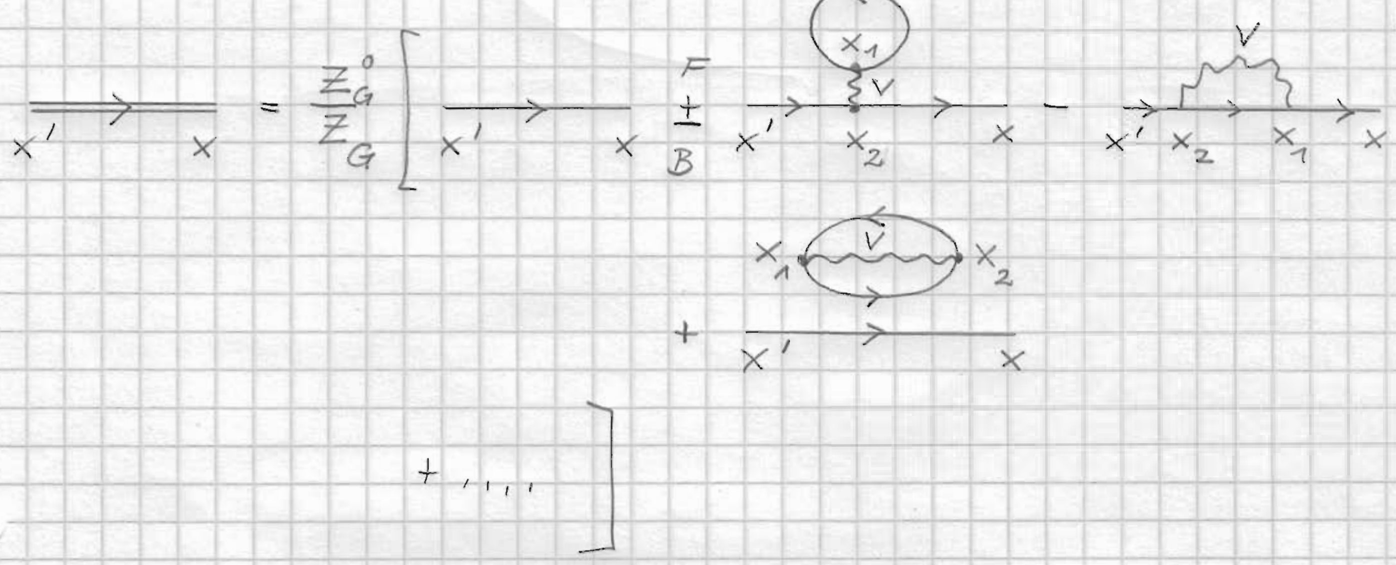
expansion of $S(\beta)$ — commutation of operators

$$+ (-1) \int d^4x_1 \int d^4x_2\, G_0(x,x_2)\, G_0(x_2,x_1)\, G_0(x_1,x') V(x_1-x_2) \qquad (B)$$

$$+ (-1)(\mp 1) \int d^4x_1 \int d^4x_2\, G_0(x,x')\; V(x_1-x_2)\; G_0(x_2,x_2) G_0(x_1,x_2)$$

$$+ O(V^2) \Big]$$

These terms of $G(x,x')$ can be represented diagrammatically:



This implies the following

<u>Diagram rules (Feynman rules)</u>

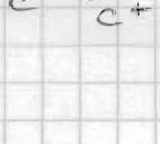
1. Denote each $G(x_1 x_2)$ by a line $\underset{x_2}{\psi^+}\longrightarrow\underset{x_1}{\psi}$.
   The arrow indicates the direction from ψ^+ to ψ, i.e. the propagation direction of an injected particle.

2. Denote each interaction $V(x_1, x_2)$ by a wavy line $\underset{x_1}{}\sim\!\sim\!\sim\underset{x_2}{}$

3. Each vertex $\underset{x_1}{\rightarrow\!\bullet\!\rightarrow}$ indicates an integration over space and time, $\int d^4x_1$, and a summation over spin (if applicable), $\sum_\sigma$.

4. Determination of sign:

- (-1) for each interaction line V from the definition and expansion of $S(\beta)$;
- for <u>fermions</u> only:
  $(-1)^p$, where p is the number of elementary commutations to bring the respective $\psi\psi^+$ pairs together to generate the respective diagram.
  This means: (-1) for each closed fermion loop.

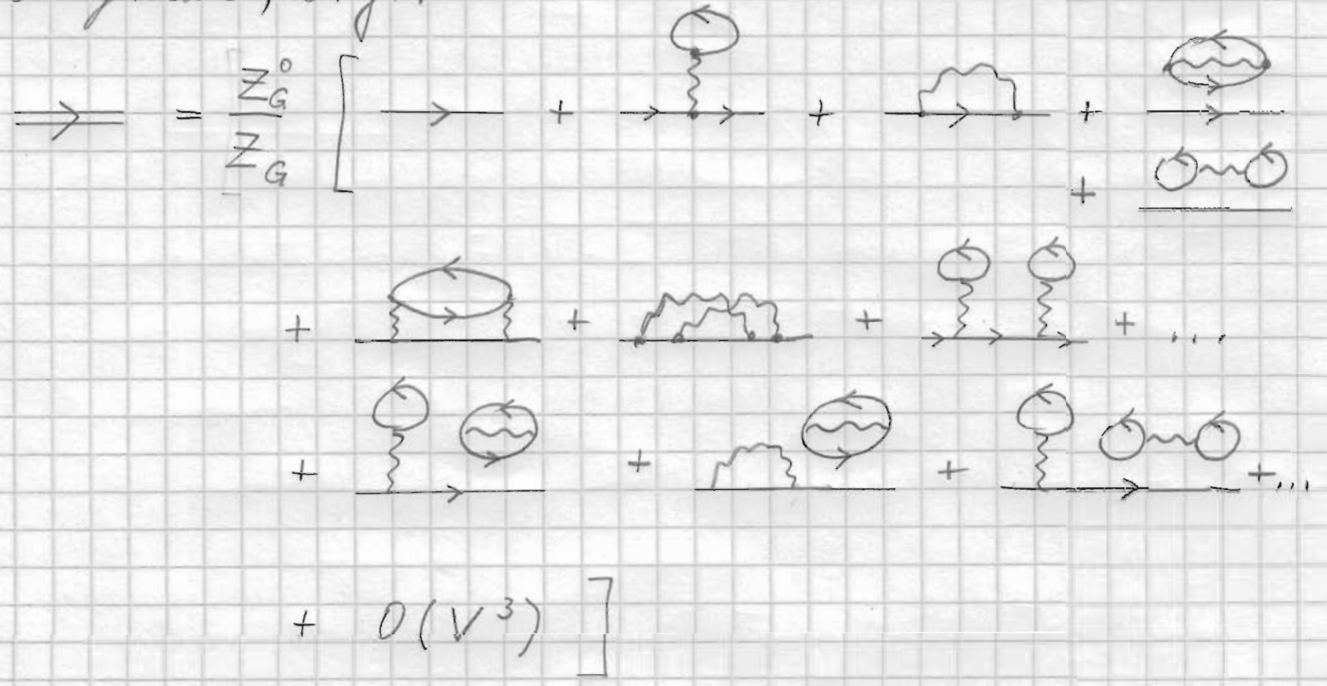
(Note: There may be different types of interactions, e.g. absorption vertices $\sim \lambda\, c^+ c\, (b + b^+)$ 

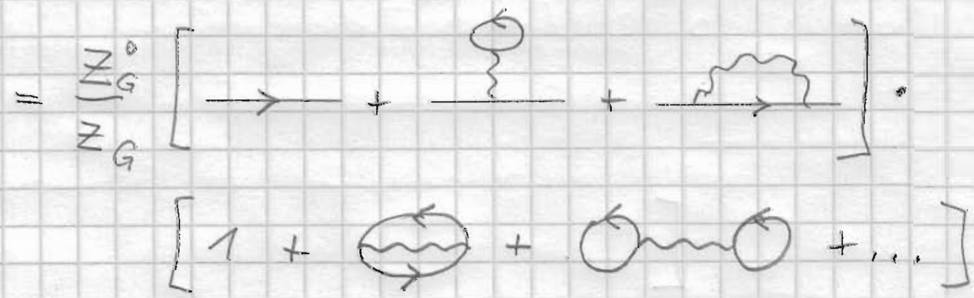
which generate different types of diagrams in an analogous way.)

5. All topologically different diagrams contribute to $G(x, x')$ with the same weight 1:
<u>Proof</u>:
The terms of n-th order perturbation theory contain exactly n interaction lines each.
They may be interchanged without changing the topology of a diagram.
From these permutations each diagram has a combinatorial factor $n!$. This factor is, however, cancelled by the factor $\frac{1}{n!}$ of the expansion of the exponential in $S(\beta)$.

6. Linked cluster theorem

The perturbation expansion contains disconnected diagrams, e.g.:





The disconnected parts of a diagram are necessarily closed diagrams, since $G(x,x')$ has exactly 2 "open ends" x, x'.
The diagrams in the 2nd bracket are exactly the ones ("closed diagrams") generated by the expansion of $\frac{Z_G}{Z_G^0}$, i.e. the 2nd bracket is cancelled by the prefactor $\frac{Z_G^0}{Z_G}$ in G.
This proves the

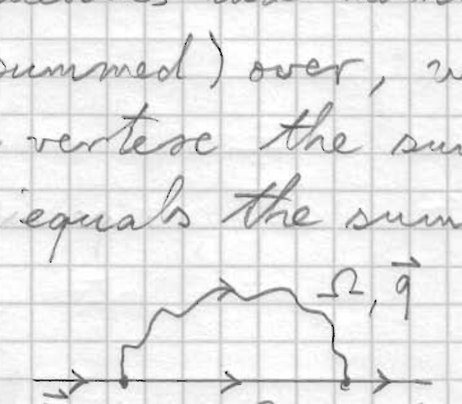
Linked cluster theorem:
Only connected diagrams contribute, and the prefactor $\frac{Z_G^0}{Z_G}$ is cancelled.

Feynman diagrams in frequency-momentum space:

The $(\omega, \vec{p})$-dependent Green's function can be represented diagrammatically by Fourier transforming $G(x, x')$ wrt. x, x' and writing $G_0(x_1, x_2)$, $V(x_1 - x_2)$ in terms of their Fourier transforms,

$$G(x_1, x_2) = \int \frac{d^3p}{(2\pi)^3} \beta \sum_{\omega_n} e^{i\vec{p}(\vec{r}_1 - \vec{r}_2) - i\omega_n(\tau_1 - \tau_2)} G_{\vec{p}}(\omega_n) .$$

The internal space-time integrals, $\int d^4x_1$ etc., then imply the energy-momentum conservation at each vertexe:
For a diagram in 4-momentum space, all internal frequencies and momenta are integrated (summed) over, with the constraint that at each vertexe the sum of in-going 4-momenta equals the sum of outgoing momenta.
Example:

$\beta \sum_{\Omega_n} \int \frac{d^3q}{(2\pi)^3}$ 

1.4.4 Selfenergy and the Dyson equation

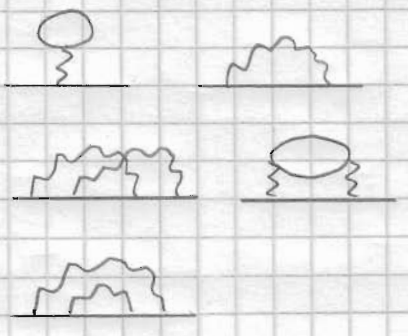
A finite sum of perturbative contributions to G does in general not preserve the analyticity (causality) of G.

In order to perform infinite summations in a controlled way, we classify all diagrams contributing to G in terms of "irreducible" and "reducible" diagrams:

Definition: irreducible diagram:
cannot be cut in 2 pieces by cutting a single G-function line.

Examples:

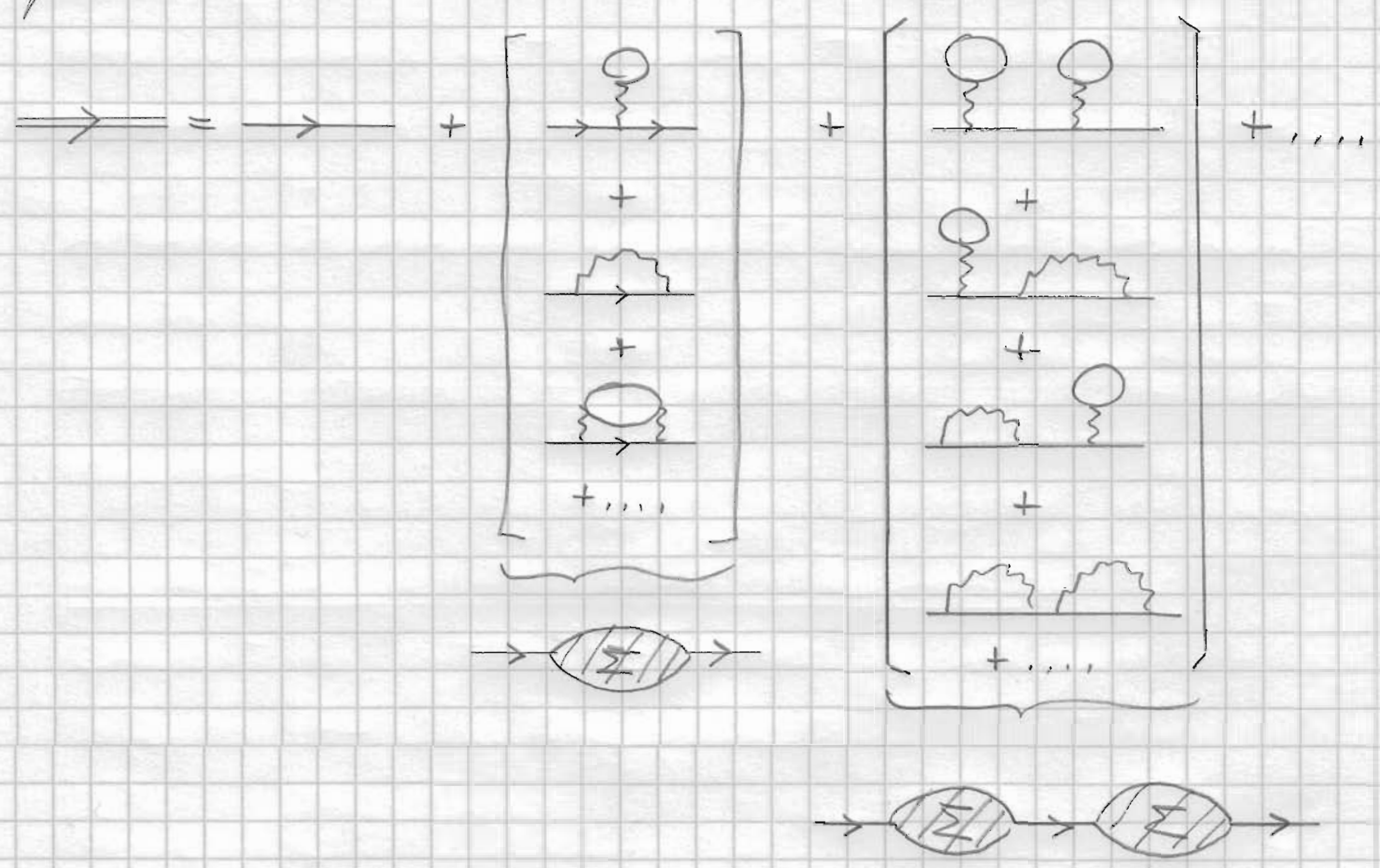
irreducible:



reducible:

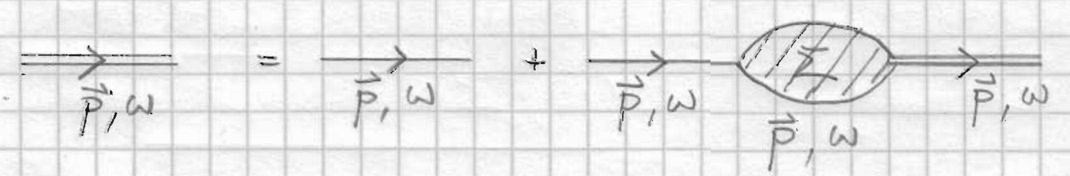
Definition:
The selfenergy $\Sigma_p(\omega)$ is the sum of all irreducible diagrams with the open-end G-function lines removed.

The diagrams contributing to G can then be classified in terms of their number of irreducible parts:



The sum in the horizontal direction can be closed as

position space



energy-momentum space

That means ,

$$\boxed{\begin{aligned} G(x,x') &= G_0(x,x') + \int d^4x_1 \int d^4x_2\, G_0(x,x_1)\,\Sigma(x_1,x_2)\,G(x_2,x') \\ G_{\vec{p}}(\omega) &= G_{0\vec{p}}(\omega) + G_{0p}(\omega)\,\Sigma_{\vec{p}}(\omega)\,G_p(\omega) \end{aligned}}$$

Dyson equation
in position space and
in 4-momentum space

Energy - momentum conservation implies that in 4 - momentum space the Dyson equation is algebraic.

It can be solved easily with

$$G_{0\vec{p}}(\omega_n) = \frac{1}{i\omega + \mu - \varepsilon_p}$$

$$G^{R/A}_{\vec{p}}(\omega)_n = \frac{G^0}{1 - G^0\Sigma} = \frac{1}{i\omega_n + \mu - \varepsilon_p - \Sigma_p(\omega_n)}$$

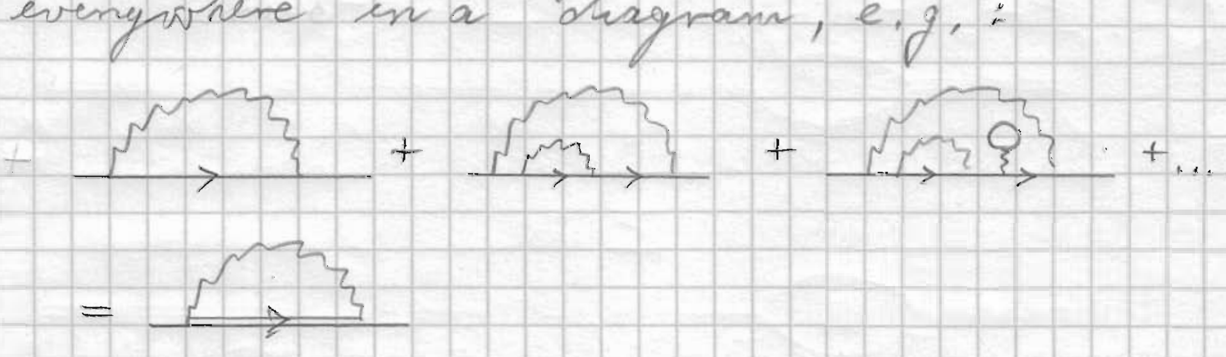
- The problem is reduced to calculating the irreducible parts Σ .
- The form of $G_{\vec{p}}(\omega_n)$ justifies the name "selfenergy Σ" for the sum of irreducible parts.

- $\Sigma_p(z)$ determines the position of the poles of $G_p(z)$. It can be shown that it shifts the poles of $G_p^{R/A}(z)$ to the lower / upper half plane only, i.e. <u>causality is preserved</u>, and $\tilde{\varepsilon}_p$, γ, and Z_p are deduced from Σ as in 1.3.2

- The Dyson equation enables us to sum up infinite series of irreducible contributions, while preserving causality.
It suggests controlled approximations for the irreducible part Σ.

1.4.5 <u>Selfconsistent approximations</u>

The sum of <u>all</u> selfenergy insertions in a diagram can be performed by replacing $G_0 \to G$ everywhere in a diagram, e.g.:



<u>Definition</u>: A diagram without selfenergy insertions is called <u>skeleton diagram</u> (i.e. without "muscles").

It follows that the selfenergy Σ is the sum of all irreducible skeleton diagrams, with each Green's function line G_0 replaced by the full, renormalized Green's function G.
Hence, the selfenergy is a functional of the full Green's function G:

$$\boxed{\begin{aligned} \Sigma_{\vec{p}}(\omega) &= \Sigma\{G\} \qquad \text{with} \\ G_{\vec{p}}(\omega) &= \frac{1}{\omega+\mu-\varepsilon_{p}-\Sigma_{\vec{p}}(\omega)} \end{aligned}}$$

Since the selfenergy involves calculating the full G-function, which in turn requires the knowledge of Σ, this is a <u>selfconsistent</u> set of equations. It is usually solved by iteration.

Selfconsistent approximations are generated by defining an approximate functional $\Sigma\{G\}$, e.g. by taking a finite order of skeleton diagrams.

<u>Example</u>: selfconsistent Hartree-Fock:

$\Sigma =$  $+$  1st order in V.

Remark (without proof):

How is the approximate $\Sigma\{G\}$ to be chosen in an "optimal" way?
So-called conserving approximations are generated by deriving Σ from a generating functional $\Phi\{G\}$ by functional derivative:

$$\Sigma\{G\} = \frac{\delta \Phi\{G\}}{\delta G}$$

Where Φ is a sum of closed skeleton diagrams.