2.3.6 Many-body perturbation theory (MBPT)

MBPT is a systematic approach by expanding the G_n as a power series ("brute force") in a part (typically the interaction) of a Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_{int}$:

$$G_n = \frac{1}{i^n} \frac{\mathrm{Tr}\left[\mathcal{T}\{e^{-i\int_\gamma d\bar{z}\,\hat{H}_0(\bar{z}) - i\int_\gamma d\bar{z}\,\hat{H}_{int}(\bar{z})}\,\hat{\varphi}(1)\ldots\hat{\varphi}^+(1')\}\right]}{\text{same as numerator but without } \hat{\varphi}\ldots\hat{\varphi}^+}$$

where we used that $\hat{H}_0$ and $\hat{H}_{int}$ commute under the $\mathcal{T}$.

Expansion in powers of $\hat{H}_{int}$:

$$G_n = \frac{1}{i^n} \frac{\sum_{k=0}^{\infty} \frac{(-i)^k}{k!} \int d\bar{z}_1 \ldots d\bar{z}_k \left\langle \mathcal{T}\left\langle \hat{H}_{int}(\bar{z}_1)\ldots\hat{H}_{int}(\bar{z}_k)\,\hat{\varphi}(1)\ldots\hat{\varphi}^+(1')\right\}\right\rangle_0}{\text{same as numerator but without } \hat{\varphi}\ldots\hat{\varphi}^+}$$

with $\langle \mathcal{T}\{\ldots\}\rangle_0 \equiv \mathrm{Tr}\left[\mathcal{T}\{e^{-i\int_\gamma d\bar{z}\,\hat{H}_0(\bar{z})}\ldots\}\right]$.

As before we consider a general 2-body interaction

$$\hat{H}_{int}(z) = \frac{1}{2}\int dz' \int dx dx'\, v(x,z;x',z')\,\hat{\varphi}^+(x,z^+)\hat{\varphi}^+(x',z'^+)\hat{\varphi}(x',z')\hat{\varphi}(x,z)$$

with $v(x,z;x',z') = \delta(z,z') \begin{cases} v(x,x',t) & \text{if } z = t_\pm \\ v^M(x,x') & \text{if } z = -i\tau. \end{cases}$

Using $a \equiv (x_a, z_a)$ and $b \equiv (x_b, z_b)$, and renaming $\bar{z}_k \to z_k$, we have for $n=1$

$$G(a,b) = \frac{1}{i} \frac{\sum_{k=0}^{\infty} \frac{(-i)^k}{k!} \int dz_1 \ldots dz_k \left\langle \mathcal{T}\{\hat{H}_{int}(z_1)\ldots\hat{H}_{int}(z_k)\,\hat{\varphi}(a)\,\hat{\varphi}^+(b)\}\right\rangle_0}{\text{same without } \hat{\varphi}(a)\,\hat{\varphi}^+(b)}$$

Now we write the numerator using the specific form of $\hat{H}_{int}$:

$$\sum_{k=0}^{\infty} \frac{1}{k!}\left(-\frac{i}{2}\right)^k \int d1\ldots dk\, d1'\ldots dk'\, v(1;1')\ldots v(k;k') \times$$

$$\times \left\langle \mathcal{T}\left\{ \hat{\Psi}^+(1^+)\hat{\Psi}^+(1'^+)\hat{\Psi}(1')\hat{\Psi}(1)\ldots\hat{\Psi}^+(k^+)\ldots\Psi^+(k'^+)\Psi(k')\hat{\Psi}(k)\,\hat{\Psi}(a)\hat{\Psi}^+(b)\right\}\right\rangle_0 .$$

Reordering:

$$\left\langle \mathcal{T}\left\{\hat{\Psi}(a)\Psi(1)\hat{\Psi}(1')\ldots\Psi(k)\Psi(k')\hat{\Psi}^+(k'^+)\hat{\Psi}^+(k)\ldots\hat{\Psi}^+(1'^+)\hat{\Psi}^+(1^+)\hat{\Psi}^+(b)\right\}\right\rangle_0 ,$$

Which we identify as

$$i^{2k+1} Z_0\, G_{0,2k+1}(a,1,1',\ldots,k,k';b,1^+,1'^+,\ldots,k^+,k'^+),$$

whereas the denominator in the k-th order term is

$$i^{2k} Z_0\, G_{0,2k}(1,1',\ldots,k,k';1^+,1'^+,\ldots,k^+,k'^+).$$

$$\Rightarrow G(a;b) = \frac{\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i}{2}\right)^k \int v(1;1')\ldots v(k;k')\, G_{0,2k+1}(a,1,1',\ldots;b,1^+,1'^+,\ldots)}{\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i}{2}\right)^k \int v(1;1')\ldots v(k;k')\, G_{0,2k}(1,1',\ldots;1^+,1'^+\ldots)}$$

where $\int\ldots \equiv \int d1\ldots dk\, d1'\ldots dk' \ldots$

Now we can apply Wick's theorem and arrive at:

$$G(a;b) = \frac{\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i}{2}\right)^k \int v(1;1')\ldots v(k;k') \begin{vmatrix} G_0(a;b) & G_0(a;1^+) & \ldots & G_0(a;k'^+) \\ G_0(1;b) & G_0(1;1^+) & \ldots & G_0(1;k'^+) \\ \vdots & \vdots & & \vdots \\ G_0(k';b) & G_0(k';1^+) & \ldots & G_0(k';k'^+) \end{vmatrix}_{\pm}}{\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i}{2}\right)^k \int v(1;1')\ldots v(k;k') \begin{vmatrix} G_0(1;1^+) & G_0(1;1'^+) & \ldots & G_0(1;k'^+) \\ G_0(1';1^+) & G_0(1';1'^+) & \ldots & G_0(1';k'^+) \\ \vdots & \vdots & & \vdots \\ G_0(k';1^+) & G_0(k';1'^+) & \ldots & G_0(k';k'^+) \end{vmatrix}_{\pm}} \qquad (*)$$

which provides an exact expansion of G in terms of G_0.

Note: Convergence and thus existence of the Taylor series is assumed here. In practice it needs to be checked for the concrete problem under consideration.

2.3.6.1 Getting started with Feynman diagrams

Feynman 1948: Invention of his famous Feynman diagrams to represent each term in the expansion graphically.

The denominator of (*) – the expression of $G(a;b)$ – is the ratio Z/Z_0 = interacting partition function / noninteracting part. fct.

To first order in v (interaction) this is:

$$\left(\frac{Z}{Z_0}\right)^{(1)} = \frac{i}{2}\int d1\,d1'\, v(1;1') \begin{vmatrix} G_0(1;1^+) & G_0(1;1'^+) \\ G_0(1';1^+) & G_0(1';1'^+) \end{vmatrix}_{\pm} = \frac{i}{2}\int d1\,d1'\, v(1;1')\left[G_0(1;1^+)G_0(1';1'^+) \pm G_0(1;1'^+)G_0(1';1^+)\right]$$

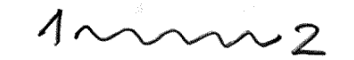
Here we introduce the basic Feynman diagrams = "lego blocks" from which all of the more complicated diagrams can be constructed:

$G_0(1;2^+)$ = 

destroy at 1 — create at 2

direction is to distinguish from $G_0(2;1^+)$; the "+" only matters when $t_1 = t_2$.

Read as "particle is created at 2, propagates and gets destroyed at 1"

$v(1;2)$ = 

$= v(2;1)$ interaction acting between 1 and 2 (or symmetrically between 2 and 1).

Two terms in $\left(\frac{Z}{Z_0}\right)^{(1)}$:

Here integration over internal vertices 1 and 1' is implied.

These diagrams correspond to the Hartree-Fock approximation but with $G \to G_0$.

Convention: When we omit the "+" shift and a diagram contains a G with same contour-time arguments, then the second argument is understood to be infinitesimally later ("+") than the first.

Here the prefactor is $\left(\frac{i}{2}\right)$ for the first diagram and $\left(\pm\frac{i}{2}\right)$ for the second one.

2nd order in v: perm./det. of 4×4 matrix $\Rightarrow 4!=24$ terms

$$\left(\frac{Z}{Z_0}\right)^{(2)} = \frac{1}{2!}\frac{i^2}{2^2}\int d1\,d1'\,d2\,d2'\,v(1;1')\,v(2;2')\sum_P (\pm)^P G_0(1;P(1))\,G_0(1';P(1'))\,G_0(2;P(2))\,G_0(2';P(2'))$$

Vacuum diagrams: only internal vertices, that are integrated over

Also called "closed diagrams".

Rules to convert vacuum diagrams into mathematical expressions:

- number all vertices and assign an interaction line $v(i;j)$ to a wiggly line between i and j and a Green's function $G_0(i;j'^+)$ to an oriented line from j to i,
- integrate over all vertices and multiply by $\left[(\pm)^P\frac{1}{k!}\left(\frac{i}{2}\right)^k\right]$, where $(\pm)^P$ is the sign of the permutation of vertex indices and k is the number of interaction (wiggly) lines.

Non-vacuum diagrams:

Now consider the numerator of $(*)$, which we call $N(a;b)$.

First order: 3×3 matrix.

$$N^{(1)}(a;b) = \frac{i}{2} G_0(a;b) \int d1\,d1'\, v(1;1') \begin{vmatrix} G_0(1,1^+) & G_0(1;1'^+) \\ G_0(1';1^+) & G_0(1';1'^+) \end{vmatrix}_{\pm}$$

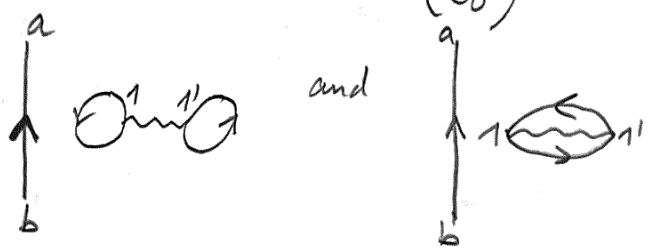
$$\pm \frac{i}{2} \int d1\,d1'\, v(1;1')\, G_0(1;b) \begin{vmatrix} G_0(a;1) & G_0(a;1'^+) \\ G_0(1';1^+) & G_0(1';1'^+) \end{vmatrix}_{\pm}$$

$$\pm \frac{i}{2} \int d1\,d1'\, v(1;1^+)\, G_0(1';b) \begin{vmatrix} G_0(a;1^+) & G_0(a;1'^+) \\ G_0(1;1^+) & G_0(1;1'^+) \end{vmatrix}_{\pm}.$$

Quiz: Do you recognize what the first line represents? Draw the two diagrams. What is the permutation of second indices?

Answer: The first line represents $G_0(a;b) \times \left(\frac{\Sigma}{\Sigma_0}\right)^{(1)}$.

The diagrams are



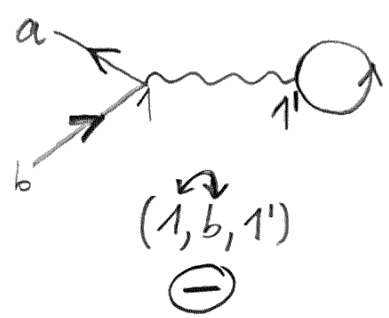
permutation P: $(b, 1, 1')$ (= identity permutation)

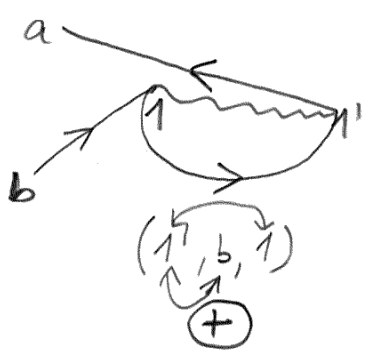
applied to $(b,1,1')$, the second indices for first indices $(a,1,1')$

$(b, 1', 1)$ one crossing $\Rightarrow$ minus sign

Quiz: Do the same for the second and third line.

Answer:





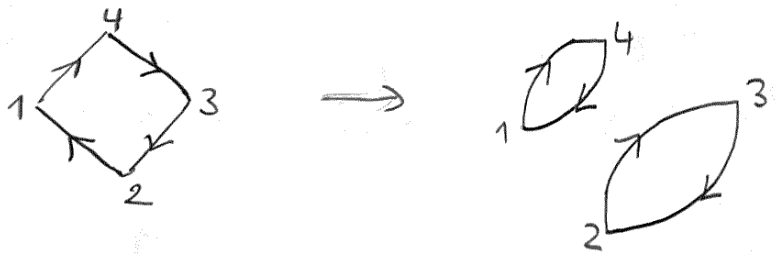
These are Green's function diagrams (no integration over external indices).
How to simply determine the sign of a permutation?
This brings us to the ...

2.3.6.2 Loop rule

The sign of a diagram is related to the sign of a permutation that changes the 2nd argument (starting point) of the corresponding Green's function.

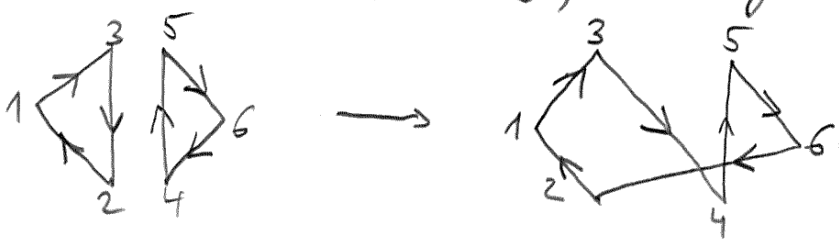
Vacuum diagrams consist of loops:
Interchange of labels (i,j) can occur either between two starting points of the same loop or between two starting points of different loops.

Case (i): same loop. E.g., interchange $2 \leftrightarrow 4$ in



$\Rightarrow$ # loops (number of loops) increases by 1.

Case (ii): different loops. E.g., interchange 3 and 6 in



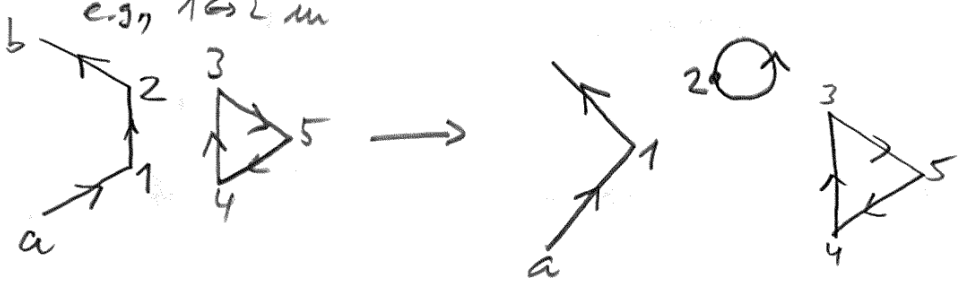
$\Rightarrow$ # loops decreases by 1.

General rule: # loops changes by ± 1 for one interchange of starting points (second 6 arguments).

For G-diagrams, there are two additional possibilities:

(iii) interchange between starting points on $a \to b$ path

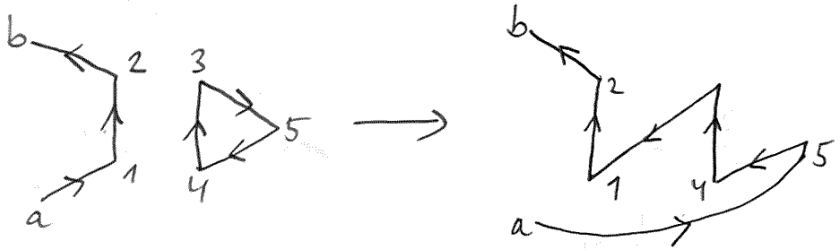
e.g., $1 \leftrightarrow 2$ in



$\Rightarrow$ # loops increases by 1

(iv) interchange between one starting point on $a \to b$ path and one starting point on a loop (internal):

e.g., $a \leftrightarrow 3$ in



$\Rightarrow$ # loops decreases by 1.

The identity permutation has sign + by definition.

$\Rightarrow$ **loop rule:** $\pm P = (\pm)^{\ell}$ with $\ell =$ # loops in a diagram

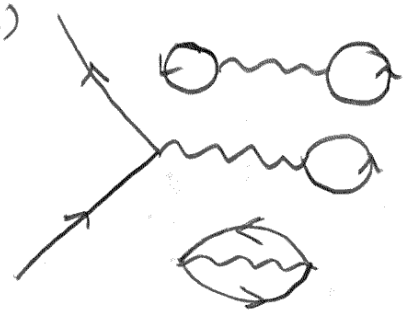
2.3.6.3 Cancellation of disconnected diagrams

The disconnected vacuum diagrams in the numerator are exactly cancelled by the vacuum diagrams in the denominator.

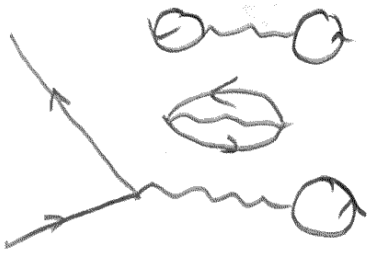
Example: some third order terms in the numerator

(1)

(2)



(3)

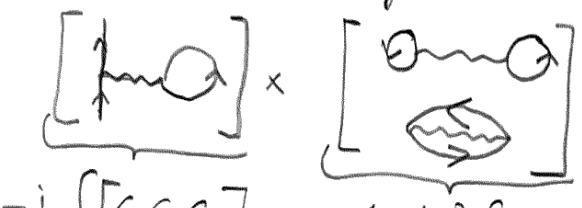


Clearly (1), (2) and (3) are interrelated by the permutation of interaction lines $v(i;i') \leftrightarrow v(j;j')$ preserving the structure of disjoint pieces. They also all have the same prefactor $(\pm)^4 \frac{1}{3!} \left(\frac{i}{2}\right)^3$.

Their total contribution thus is:

$$3 \times \frac{1}{3!} \left(\frac{i}{2}\right)^3 \underbrace{\int [G_0 G_0 G_0 v]}_{G\text{-diagram}} \underbrace{\int [G_0 G_0 G_0 G_0 vv]}_{\text{vacuum diagram}}$$

Now consider the product



$$-\frac{1}{2} \int [G_0 G_0 G_0 v] \qquad -\frac{1}{2!} \left(\frac{i}{2}\right)^2 \int [G_0 G_0 G_0 G_0 vv]$$

} = same as the 3 diagrams above!

This argument can be generalized to all diagrams — see Stefanucci & van Leeuwen, Chapter 10.3.

Let us denote by $G_c^{(n)}(a;b)$ the sum of all n-th order connected diagrams of $N(a;b)$:

$$G_c^{(n)}(a,b) = \frac{1}{n!}\left(\frac{i}{2}\right)^n \sum_{\substack{i = G\text{-connected} \\ \text{diagrams}}} (\pm)^{k_i}\, G_{c,i}^{(n)}(a;b)$$

Then one can show that

$$N(a;b) = \sum_{k=0}^{\infty}\sum_{n=0}^{k} G_c^{(n)}(a;b)\left(\frac{Z}{Z_0}\right)^{(k-n)} \overset{\text{shift of indices}}{=} \sum_{n=0}^{\infty}\sum_{k=n}^{\infty} G_c^{(n)}(a;b)\left(\frac{Z}{Z_0}\right)^{(k-n)}$$

$$= \boxed{\left(\frac{Z}{Z_0}\right)} \sum_{n=0}^{\infty} G_c^{(n)}(a;b).$$

$\Rightarrow$ "cancellation of disconnected diagrams" between numerator $N(a;b)$ and denominator $\left(\frac{Z}{Z_0}\right)$.

Result: G can be computed from a sum of <u>connected</u> diagrams only!

$$G(a;b) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{i}{2}\right)^n \int v(1;1')\ldots v(n;n') \begin{vmatrix} G_0(a;b) & G_0(a;1+) & \ldots & G_0(a;n'+) \\ G_0(1;b) & G_0(1;1+) & \ldots & G_0(1;n'+) \\ \vdots & \vdots & & \vdots \\ G_0(n';b) & G_0(n';1+) & \ldots & G_0(n';n'+) \end{vmatrix}_{\pm c}$$

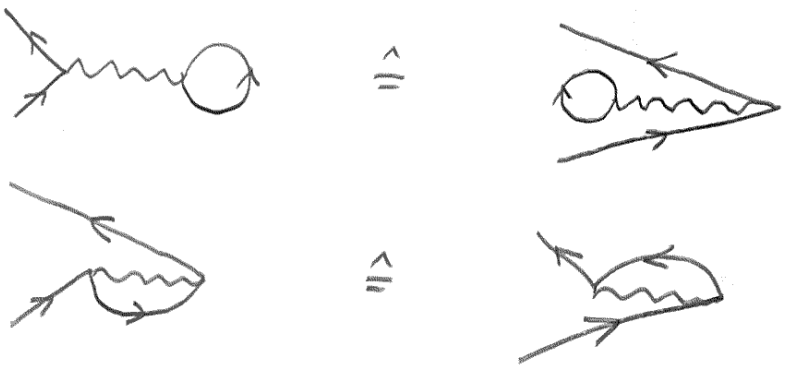
2.3.6.4 Summing only topologically inequivalent diagrams

[Details: Stefanucci & van Leeuwen, Chap. 10.4]

$$G(a;b) = \sum_{n=0}^{\infty} i^n \int v(1;1') \dots v(n;n') \begin{vmatrix} G_0(a;b) & G_0(a;1^+) & \dots & G_0(a;n'^+) \\ G_0(1;b) & G_0(1;1^+) & \dots & G_0(1;n'^+) \\ \vdots & & & \vdots \\ G_0(n';b) & G_0(n';1^+) & \dots & G_0(n';n'^+) \end{vmatrix}^{\pm}_{\text{top.ineq.}}$$

It turns out that one can get rid of the combinatorial prefactor $\left(\frac{1}{2}\right)^n \frac{1}{n!}$ by considering only "topologically inequivalent" diagrams. These are diagrams that cannot be continuously deformed into one another by mirroring or interchanging interaction lines.

Example for topo-equivalent diagrams from before:



$\Rightarrow$ one of the equivalent diagrams can be obtained from the other by mirroring the 1 and 1' in $v(1;1')$.

Fun fact: There are precisely 2^n mirrored configurations at order n, and precisely $n!$ permutations of wiggly lines.

$\Rightarrow$ Consider only diagrams with distinct topology and multiply by $2^n n!$, where n is the number of (wiggly) interaction lines.

$\Rightarrow$ new value of prefactor becomes $2^n n! \frac{1}{n!} \left(\frac{i}{2}\right)^n (\pm)^l = i^n (\pm)^l$

$$\Rightarrow \boxed{G(a;b) = \sum_{n=0}^{\infty} i^n \int v(1;1') \ldots v(n;n') \begin{vmatrix} G_0(a;b) & G_0(a;1') & \ldots & G_0(a;n') \\ G_0(1;b) & G_0(1;1') & \ldots & G_0(1;n') \\ \vdots & \vdots & & \vdots \\ G_0(n;b) & G_0(n;1') & \ldots & G_0(n;n') \end{vmatrix}_{\substack{\pm \\ c \\ \text{topo. ineq.}}}}$$

where the symbol $|\ldots|_{\substack{\pm \\ c \\ \text{topo. ineq.}}}$ signifies that we retain from the permanent / determinant only connected and only one of each possible topologically equivalent (i.e., only topologically inequivalent) diagrams.

New rules for converting a diagram into a mathematical expression:

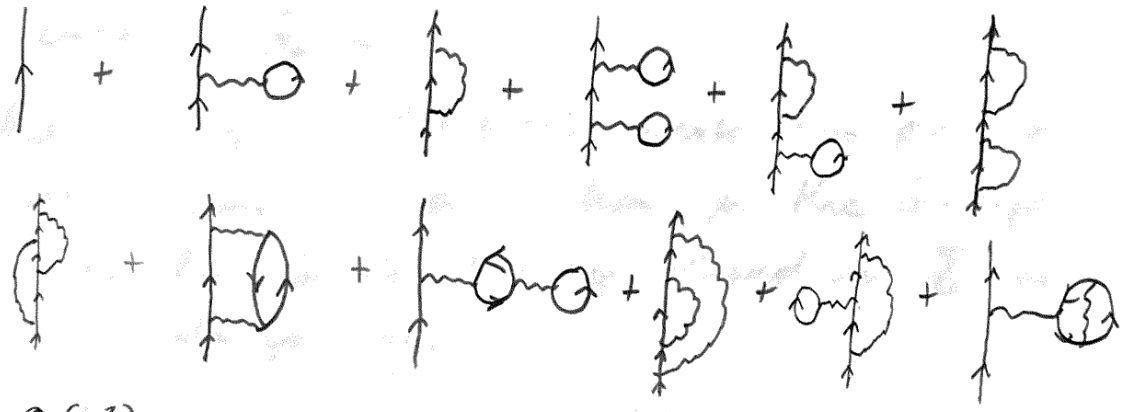
- number all vertices and assign an interaction line $v(i;j)$ to a wiggly line between j and i and a Green's function $G_0(i;j')$ to an oriented line from j to i.
- integrate over all internal vertices and multiply by $i^n (\pm)^l$, where l is the number of loops and n is the number of interaction lines.

=> using these rules we can expand $G(a;b)$ to second order. We find <u>two</u> first-order diagrams and <u>ten</u> second-order diagrams.

<u>Note</u>: Without the cancellation of disconnected diagrams and resummation of topologically equivalent diagrams the G to second order would consist of 169 diagrams.

12 versus 169 = enormous simplification!

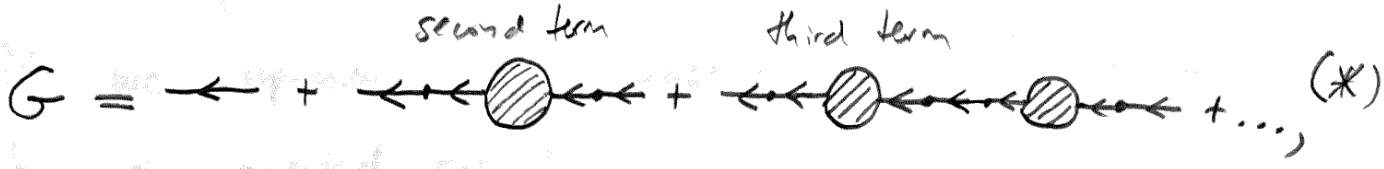
Up to second order MBPT we thus have

$G =$ 

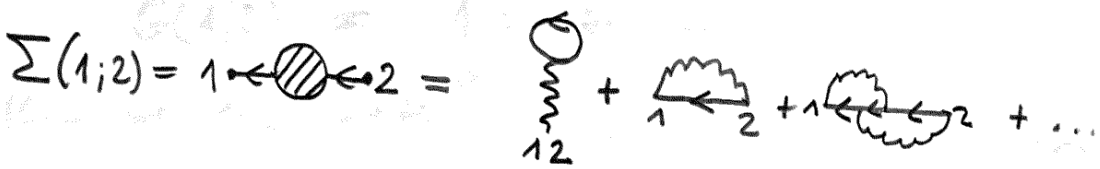
$+ \mathcal{O}(v^3)$

2.3.6.5 Self-energy and Dyson equations

From the diagrammatic structure it is clear that G has the form



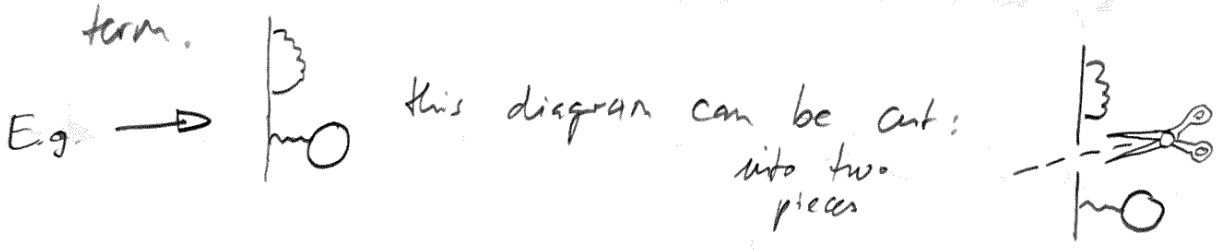
with the self-energy Σ:

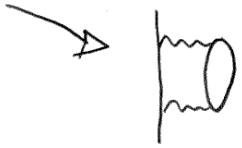


Σ = all diagrams in between ← ... ← in the G-expansion that do <u>not</u> break up into two disjoint pieces when one cuts a G_0-line.

Why? Answer: Diagrams that break create two pieces that themselves come from a Σ term in the G-expansion, so pieces that break are not allowed in Σ to avoid double counting.

Examples: In the second-order MBPT diagrams for G (p. 40) all of the diagrams in the first row that are of order V^2 are part of the third term on the rhs. (*), while the diagrams in the second row are part of the second term.





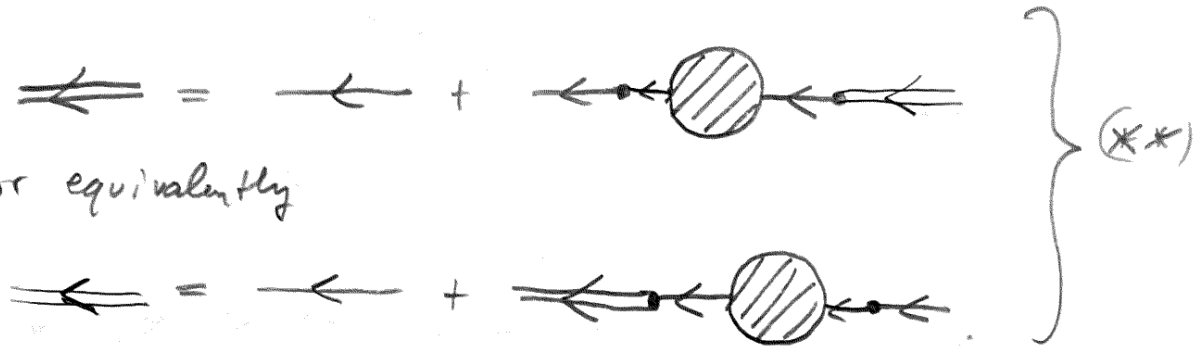
The Σ diagrams are called (one-particle) irreducible diagrams.

$\Sigma = \Sigma[G_0, V]$ is a <u>functional</u> of the noninteracting Green's function G_0 and the interaction V.

If we represent the interacting Green's function G by an oriented double line

$G(1;2) =$ 

then we can write



or equivalently

<u>Quiz</u>: Show that either of the two representations of G in $(**)$ are equivalent to $(*)$.

<u>Answer:</u> Iterate for instance the upper line in $(**)$:

$$G = G_0 + G_0 \Sigma G = G_0 + G_0 \Sigma [G_0 + G_0 \Sigma G] = G_0 + G_0 \Sigma G_0 + \dots$$

$$\dots + G_0 \Sigma G_0 \Sigma [G_0 + G_0 \Sigma G] = \text{same as } (*).$$

Alternative way to understand the equivalence: Geometric series.

$$G = G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 + \dots$$

$$= G_0 \left(1 + \Sigma G_0 + \Sigma G_0 \Sigma G_0 + \dots\right) = G_0 \sum_{n=0}^{\infty} (\Sigma G_0)^n = \dots$$

Geo. series: $\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \Rightarrow \dots = G_0 \frac{1}{1 - \Sigma G_0} \Rightarrow G^{-1} = G_0^{-1} - \Sigma$

And (**) implies $G = G_0 + G_0 \Sigma G$, which can be solved for G formally as $G^{-1} = G_0^{-1} - \Sigma$, the same as the result of the geometric series.

Note: This is a handwaving argument here since in reality we are dealing with integral equations. ← but instructive!

(**) really means

$$\boxed{G(1;2) = G_0(1,2) + \int d3\, d4\; G_0(1;3)\, \Sigma(3;4)\, G(4;2)}$$

Dyson equation.

The Dyson equation can be shown to be equivalent to the integro-differential equations called Kadanoff-Baym equations (derived in 2.3.4 for the Hartree-Fock self-energy):

$$\boxed{\begin{aligned} \left[i\frac{d}{dz_1} - h(1) \right] G(1;1') &= \delta(1;1') + \int d2\; \Sigma(1;2)\, G(2;1') \\ G(1;1') \left[-i\frac{\overleftarrow{d}}{dz_1'} - h(1') \right] &= \delta(1;1') + \int d2\; G(1;2)\, \Sigma(2;1') \end{aligned}}$$

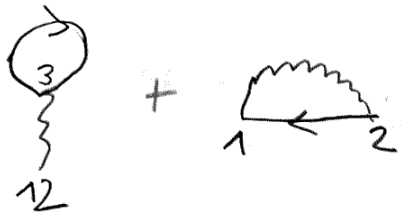
+ KMS boundary conditions.

Difference: In the Dyson equation the KMS conditions are automatically incorporated via G_0 — if G_0 fulfills KMS, then G also does.

Also, the information about the single-particle h is also contained in the noninteracting G_0.

The rules to construct and mathematically interpret diagrams for Σ are analogous to those for G.

E.g., to first order we have

$\Sigma^{(1)}(1;2) =$ 

$$= \pm i \delta(1;2) \int d3\, v(1;3) G_0(3;3^+) + i v(1;2) G_0(1;2^+)$$

δ-function for all Σ diagrams that start and end with the same index (here $1=2$).

To second order we have

$\Sigma^{(2)}(1;2) =$