

Lecture on First-principles Computations (22)

Evaluation of the Interacting Green Function

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Recall: properties of the Green function

- Defined as the expectation value of the time-ordered product of creation and destruction operators with respect to the exact ground state.
- Once known, can be used to compute
 - the expectation value of any single-particle operator within the ground state of the system
 - the ground-state energy
(through the equation of motion of the Green function)
 - the excitation spectrum of the system
(through the Lehmann representation)

How to evaluate the Green function for interacting systems ?

The usual approach is the perturbation theory.
For this it is most convenient to work in **the
interaction picture !**

The interaction picture

- Schrödinger picture:
$$i \frac{\partial |\Psi_S(t)\rangle}{\partial t} = \hat{H} |\Psi_S(t)\rangle$$

$$|\Psi_S(t)\rangle = e^{-i\hat{H}(t-t_0)} |\Psi_S(t_0)\rangle, \quad O(t) = \langle \Psi_S(t) | \hat{O}_S | \Psi_S(t) \rangle$$

- Heisenberger Picture:
$$|\Psi_H(t)\rangle = e^{i\hat{H}t} |\Psi_S(t)\rangle = |\Psi_S(0)\rangle$$

$$i \frac{\partial |\Psi_H(t)\rangle}{\partial t} = 0, \quad \hat{O}_H(t) = e^{i\hat{H}t} \hat{O}_S e^{-i\hat{H}t}$$

- The interaction picture:
$$\hat{H} = \hat{H}_0 + \hat{H}_{int}$$

$$|\Psi_I(t)\rangle = e^{i\hat{H}_0 t} |\Psi_S(t)\rangle, \quad i \frac{\partial |\Psi_I(t)\rangle}{\partial t} = \hat{H}_{int}(t) |\Psi_I(t)\rangle$$

$$\hat{O}_I(t) = e^{i\hat{H}_0 t} \hat{O}_S e^{-i\hat{H}_0 t}, \quad \hat{H}_{int}(t) = e^{i\hat{H}_0 t} \hat{H}_{int} e^{-i\hat{H}_0 t}$$

$$i \frac{\partial \hat{O}_I(t)}{\partial t} = [\hat{O}_I(t), \hat{H}_0]$$

The evolution operator in the interaction picture

The evolution operator:

$$|\Psi_I(t)\rangle = \hat{U}(t, t_0)|\Psi_I(t_0)\rangle$$

A formal solution of the evolution operator,

$$\hat{U}(t, t_0) = e^{i\hat{H}_0 t} e^{i\hat{H}(t-t_0)} e^{-i\hat{H}_0 t_0}$$

Apparently $\hat{U}(t, t_0)$ is a unitary operator

$$\hat{U}^\dagger(t, t_0) = \hat{U}^{-1}(t, t_0)$$

$$\hat{U}(t_1, t_2)\hat{U}(t_2, t_3) = \hat{U}(t_1, t_3)$$

$$\hat{U}(t, t_0)\hat{U}(t_0, t) = 1$$

Integral equation of the evaluation operator

$\hat{U}(t, t_0)$ satisfy the equation of motion:

$$i \frac{\partial}{\partial t} \hat{U}(t, t_0) = \hat{H}_{int}(t) \hat{U}(t, t_0)$$

We can turn this into an integral equation:

$$\hat{U}(t, t_0) = 1 - i \int_{t_0}^t \hat{H}_{int}(t') \hat{U}(t', t_0) dt'$$

Solving the integral equation iteratively:

$$\hat{U}(t, t_0) = 1 - i \int_{t_0}^t \hat{H}_{int}(t') dt' + (-i)^2 \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \hat{H}_{int}(t') \hat{H}_{int}(t'') + \dots$$

where $\hat{H}_{int}(t) = \frac{1}{2} \int \int dx dx' \hat{\Psi}^\dagger(x, t) \hat{\Psi}^\dagger(x', t) V(x, x') \hat{\Psi}(x', t) \hat{\Psi}(x, t)$

The perturbative solution of the evaluation operator

$$\begin{aligned} \hat{U}(t, t_0) &= 1 - i \int_{t_0}^t \hat{H}_{int}(t') dt' + (-i)^2 \int_{t_0}^t dt' \int_{t_0}^{t'} d t'' \hat{H}_{int}(t') \hat{H}_{int}(t'') + \dots \\ &= 1 - i \int_{t_0}^t \hat{H}_{int}(t') dt' + \frac{(-i)^2}{2!} \int_{t_0}^t dt' \int_{t_0}^t d t'' \hat{T}[\hat{H}_{int}(t') \hat{H}_{int}(t'')] + \dots \end{aligned}$$

Changing the range of the integral

Finally

$$\begin{aligned} \hat{U}(t, t_0) &= 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^t dt_1 \dots \int_{t_0}^t dt_n \hat{T}[\hat{H}_{int}(t_1) \dots \hat{H}_{int}(t_n)] \\ &= \hat{T} e^{-i \int_{t_0}^t \hat{H}_{int}(t') dt'} \end{aligned}$$

Adiabatic “switching on”

Consider a time-dependent Hamiltonian,

$$\hat{H} = \hat{H}_0 + e^{-\epsilon|t|} \hat{H}_{int} \quad (\epsilon: \text{a small positive number})$$

When $t \rightarrow \infty$ or $-\infty$, $\hat{H} \rightarrow \hat{H}_0$

The evolution operator can still be defined!

$$|\Psi_I(t)\rangle = \hat{U}_\epsilon(t, t_0) |\Psi_I(t_0)\rangle$$

$$i \frac{\partial}{\partial t} \hat{U}_\epsilon(t, t_0) = e^{-\epsilon|t|} \hat{H}_{int}(t) \hat{U}_\epsilon(t, t_0)$$

$$\hat{U}_\epsilon(t, t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^t dt_1 \cdots \int_{t_0}^t dt_n e^{-\epsilon(|t_1| + \cdots + |t_n|)} \hat{T}[\hat{H}_{int}(t_1) \cdots \hat{H}_{int}(t_n)]$$

$\epsilon \rightarrow 0$, interaction turned on infinitely slowly, “adiabatic”.

Adiabatic “switching-on” (II)

Suppose $|\Phi_0\rangle$ is an eigenstate of \hat{H}_0 : $\hat{H}_0|\Phi_0\rangle = E_0|\Phi_0\rangle$:

For $t_0 \rightarrow -\infty$, $|\psi_s(t_0)\rangle = e^{-iE_0 t_0}|\Phi_0\rangle$, and then

$$|\Psi_I(t_0)\rangle = e^{i\hat{H}_0 t_0}|\Psi_s(t_0)\rangle = |\Phi_0\rangle \quad (t_0 \rightarrow -\infty)$$

$$i \frac{\partial |\Psi_I(t)\rangle}{\partial t} = e^{-\epsilon|t|} \hat{H}_{int}(t) |\Psi_I(t)\rangle \rightarrow 0, \quad t \rightarrow \pm\infty$$

$$|\Psi_{I,\epsilon}(t=0)\rangle = \hat{U}_\epsilon(0, -\infty)|\Phi_0\rangle \quad (|\Psi_{I,\epsilon}(t=0)\rangle \text{ may depend on } \epsilon)$$

We would like to take $\epsilon \rightarrow 0$ (adiabatically switching on the interaction), and see what happen?

$$\lim_{\epsilon \rightarrow 0} |\Psi_{I,\epsilon}(t=0)\rangle \stackrel{?}{\rightarrow} |\Psi_H\rangle = |\Psi_0\rangle$$

Gell-Mann - Low theorem

$$\lim_{\epsilon \rightarrow 0} \frac{\hat{U}_\epsilon(0, -\infty)|\Phi_0\rangle}{\langle \Phi_0 | \hat{U}_\epsilon(0, -\infty) | \Phi_0 \rangle} = \frac{|\Psi_0\rangle}{\langle \Phi_0 | \Psi_0 \rangle}$$

The numerator and denominator don't exist separately, but the limit of the ratio is well-defined.

The limit is an eigenstate of the **full** Hamiltonian :

$$\hat{H} \frac{|\Psi_0\rangle}{\langle \Phi_0 | \Psi_0 \rangle} = E \frac{|\Psi_0\rangle}{\langle \Phi_0 | \Psi_0 \rangle}$$

The expectation value of an operator in the interaction picture

Gell-Mann – Low theorem

$$\frac{\hat{U}_\epsilon(0, -\infty)|\Phi_0\rangle}{\langle\Phi_0|\hat{U}_\epsilon(0, -\infty)|\Phi_0\rangle} = \frac{|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} \quad (\text{valid for } \epsilon \rightarrow 0)$$

$$\hat{U}_\epsilon(t, t_0) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^t dt_1 \cdots \int_{t_0}^t dt_n e^{-\epsilon(|t_1|+\cdots+|t_n|)} \hat{T}[\hat{H}_{int}(t_1) \cdots \hat{H}_{int}(t_n)]$$

It is easy to prove,

$$\frac{\langle\Psi_0|\hat{O}_H(t)|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = \frac{1}{\langle\Phi_0|\hat{S}(\infty, -\infty)|\Phi_0\rangle} \times$$

$$\langle\Phi_0|\sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n e^{-\epsilon(|t_1|+\cdots+|t_n|)} \hat{T}[\hat{H}_{int}(t_1) \cdots \hat{H}_{int}(t_n) \hat{O}_I(t)]|\Phi_0\rangle$$

The expectation value of the time-ordered product of two operators

$$\frac{\langle \Psi_0 | \hat{T}[\hat{O}_H(t)\hat{O}_H(t')] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \frac{1}{\langle \Phi_0 | \hat{S}(-\infty, \infty) | \Phi_0 \rangle} \times$$

$$\langle \Phi_0 | \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n e^{-\epsilon(|t_1| + \cdots + |t_n|)} \hat{T}[\hat{H}_{int}(t_1) \cdots \hat{H}_{int}(t_n) \hat{O}_I(t)\hat{O}_I(t')] | \Phi_0 \rangle$$

$= 1$

ϵ is allowed to take the limit $\epsilon \rightarrow 0$

As an example:

$$G(x, x'; t - t') = -i \frac{\langle \Psi_0 | \hat{T}[\hat{\Psi}_H(x, t)\hat{\Psi}_H^\dagger(x', t')] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \frac{-i}{\langle \Phi_0 | \hat{S}(-\infty, \infty) | \Phi_0 \rangle} \times$$

$$\langle \Phi_0 | \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \hat{T}[\hat{H}_{int}(t_1) \cdots \hat{H}_{int}(t_n) \hat{\Psi}_I(x, t)\hat{\Psi}_I^\dagger(x', t')] | \Phi_0 \rangle$$

Now, the interacting Green function

$$G(x, t; x', t') = -i \frac{\langle \Psi_0 | T \hat{\Psi}_H(x, t) \hat{\Psi}_H^\dagger(x', t') | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

$|\Psi_0\rangle$ is not orthonormalized in general)

Switching to the interaction picture :

$$G(x, t; x', t') = -i \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^t dt_1 \cdots \int_{t_0}^t dt_n$$
$$\frac{\langle \Phi_0 | \hat{T} [\hat{H}_{int}(t_1) \cdots \hat{\Psi}_I(x, t) \cdots \hat{\Psi}_I(x', t') \cdots \hat{H}_{int}(t_n)] | \Phi_0 \rangle}{\langle \Phi_0 | \hat{S}(\infty, -\infty) | \Phi_0 \rangle}$$

$$\hat{S}(\infty, -\infty) = \lim_{\epsilon \rightarrow 0} \hat{U}_\epsilon(\infty, -\infty)$$

The first few terms ...

The numerator:

$$\begin{aligned} \tilde{G}(x, x'; t - t') &= -i \langle \Psi_0 | \hat{T} [\hat{\Psi}_H(x, t) \hat{\Psi}_H^\dagger(x', t')] | \Psi_0 \rangle = \\ &= -i \langle \Phi_0 | \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \hat{T} [\hat{H}_{int}(t_1) \cdots \hat{H}_{int}(t_n) \hat{\Psi}_I(x, t) \hat{\Psi}_I^\dagger(x', t')] | \Phi_0 \rangle \end{aligned}$$

The denominator:

$$\langle \Phi_0 | \hat{S}(\infty, -\infty) | \Phi_0 \rangle = \langle \Phi_0 | \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \hat{T} [\hat{H}_{int}(t_1) \cdots \hat{H}_{int}(t_n)] | \Phi_0 \rangle$$

Look at the numerator first ...

- The zeroth-order term (non-interacting Green function):

$$\tilde{G}^{n=0}(x, x'; t - t') = -i \langle \Phi_0 | \hat{T} [\hat{\Psi}_I(x, t) \hat{\Psi}_I^\dagger(x', t')] | \Phi_0 \rangle = G_0(x, x'; t - t')$$

The first few terms ...

- The first-order term :

$$\begin{aligned}\tilde{G}^{n=1}(x, x'; t - t') &= \\ & i \langle \Phi_0 | \int_{-\infty}^{\infty} dt_1 \hat{T} [\hat{H}_{int}(t_1) \hat{\Psi}_I(x, t) \hat{\Psi}_I^\dagger(x', t')] | \Phi_0 \rangle \\ &= i \frac{1}{2} \int_{-\infty}^{\infty} dt_1 \int d x_1 \int d x_2 V(x_1 - x_2) \times \\ & \langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_1, t_1) \hat{\Psi}^\dagger(x_2, t_1) \hat{\Psi}(x_2, t_1) \hat{\Psi}(x_1, t_1) \hat{\Psi}(x, t) \hat{\Psi}^\dagger(x', t')] | \Phi_0 \rangle \\ & \underbrace{\hspace{15em}} \\ & \text{6 fermionic operators}\end{aligned}$$

.....

The first few terms ...

- The second-order term :

$$\begin{aligned}
 \tilde{G}^{n=2}(x, x'; t - t') &= \\
 \frac{i}{2!} \langle \Phi_0 | &\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \hat{T} [\hat{H}_{int}(t_1) \hat{H}_{int}(t_2) \hat{\Psi}_I(x, t) \hat{\Psi}_I^\dagger(x', t')] | \Phi_0 \rangle \\
 &= \frac{i}{2!} \frac{1}{2^2} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int d x_1 \int d x_2 \int d x_3 \int d x_4 V(x_1 - x_2) V(x_3 - x_4) \times \\
 &\langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_1, t_1) \hat{\Psi}^\dagger(x_2, t_1) \hat{\Psi}(x_2, t_1) \hat{\Psi}(x_1, t_1) \times \\
 &\quad \hat{\Psi}^\dagger(x_3, t_2) \hat{\Psi}^\dagger(x_4, t_2) \hat{\Psi}(x_4, t_2) \hat{\Psi}(x_3, t_2) \hat{\Psi}(x, t) \hat{\Psi}^\dagger(x', t')] | \Phi_0 \rangle
 \end{aligned}$$

10 fermionic operators

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Wick's theorem

The key is to evaluating the expectation value of the time-ordered products of operators within the non-interacting ground state.

$$\langle \Phi_0 | \hat{T}[\hat{\psi}(x_1, t_1)\hat{\psi}^\dagger(x_2, t_2)\hat{\psi}^\dagger(x_3, t_3) \cdots \hat{\psi}(x_N, t_N)] | \Phi_0 \rangle$$

Wick's theorem states that this can be factorized into products of pairs; in making all possible pairings of creation and annihilated operators, each pair should be time-ordered.

Wick's theorem

Some simple rules in applying the Wick's theorem:

- The number of creation and annihilation operators must be the same.
- The anticommutation rule needs to be taken care of when moving the operators to form pairs.
- For m creation (or annihilation) operators, there are $m!$ possible ways to form pairs ($m=2n+1$ at the n -th order.)

A simple example

$$\langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_1, t_1) \hat{\Psi}^\dagger(x_2, t_2) \hat{\Psi}(x_2, t_2) \hat{\Psi}(x_1, t_1)] | \Phi_0 \rangle$$

$$= \langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_1, t_1) \hat{\Psi}(x_1, t_1)] | \Phi_0 \rangle \langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_2, t_2) \hat{\Psi}(x_2, t_2)] | \Phi_0 \rangle \\ - \langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_1, t_1) \hat{\Psi}(x_2, t_2)] | \Phi_0 \rangle \langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_2, t_2) \hat{\Psi}(x_1, t_1)] | \Phi_0 \rangle$$

$$= (-iG(x_1, x_1; t = 0^-)) (-iG(x_2, x_2; t = 0^-)) \\ - (-iG(x_1, x_2; t_2 - t_1)) (-iG(x_1, x_2; t_1 - t_2))$$

$n(x_2)$

The electron density

A simple example

$$\langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_1, t_1) \hat{\Psi}^\dagger(x_2, t_2) \hat{\Psi}(x_2, t_2) \hat{\Psi}(x_1, t_1)] | \Phi_0 \rangle$$

$$= \langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_1, t_1) \hat{\Psi}(x_1, t_1)] | \Phi_0 \rangle \langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_2, t_2) \hat{\Psi}(x_2, t_2)] | \Phi_0 \rangle$$

$$- \langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_1, t_1) \hat{\Psi}(x_2, t_2)] | \Phi_0 \rangle \langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_2, t_2) \hat{\Psi}(x_1, t_1)] | \Phi_0 \rangle$$

$$= \left(-iG(x_1, x_1; t = 0^-) \right) \left(-iG(x_2, x_2; t = 0^-) \right)$$

$$- \left(-iG(x_1, x_2; t_2 - t_1) \right) \left(-iG(x_1, x_2; t_1 - t_2) \right)$$

$n(x_2)$

The electron density

Integrating over the Coulomb interaction, $V(x_1, x_2) \delta(t_1 - t_2)$, one gets the Hartree-Fock energy.

Evaluating the first-order Green function

$$\tilde{G}^{n=1}(x, x'; t - t') = -\frac{1}{2} \int_{-\infty}^{\infty} dt_1 \int d x_1 \int d x_2 V(x_1 - x_2) \times \\ \langle \Phi_0 | \hat{T} [\hat{\Psi}^\dagger(x_1, t_1) \hat{\Psi}^\dagger(x_2, t_1) \hat{\Psi}(x_2, t_1) \hat{\Psi}(x_1, t_1) \hat{\Psi}(x, t) \hat{\Psi}^\dagger(x', t')] | \Phi_0 \rangle$$

There are **six** ways of forming pairs!

$$(1) = \left(-iG_0(x_1, x_1; 0^-)\right) \left(-iG_0(x_2, x_2; 0^-)\right) \left(iG_0(x, x'; t - t')\right)$$

$$(2) = -\left(-iG_0(x_1, x_2; 0^-)\right) \left(-iG_0(x_2, x_1; 0^-)\right) \left(iG_0(x, x'; t - t')\right)$$

$$(3) = -\left(-iG_0(x, x_1; t - t_1)\right) \left(-iG_0(x_2, x_2; 0^-)\right) \left(iG_0(x_1, x'; t_1 - t')\right)$$

$$(4) = \left(-iG_0(x_1, x_2; 0^-)\right) \left(-iG_0(x, x_1; t - t_1)\right) \left(iG_0(x_2, x'; t_2 - t')\right)$$

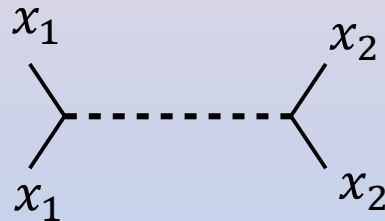
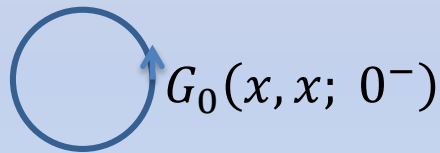
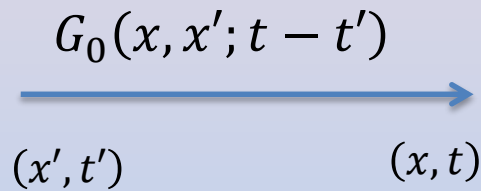
$$(5) = -\left(-iG_0(x, x_2; t - t_1)\right) \left(-iG_0(x_1, x_1; 0^-)\right) \left(iG_0(x_2, x'; t_1 - t')\right)$$

$$(6) = \left(-iG_0(x_2, x_1; 0^-)\right) \left(-iG_0(x, x_2; t - t_1)\right) \left(iG_0(x_1, x'; t_2 - t')\right)$$

It is very tedious and lengthy to evaluate these terms algebraically; not the way to go!

The way out: Feynman diagrams

Using pictures to represent the algebraical expressions!



$$V(x_1 - x_2)\delta(t_1 - t_2)$$

Advantages of Feynman diagrams:

- Intuitive, and reflects the underlying physical processes
- Reveals simple rules for accounting for physically relevant contributions.

The cancellation theorem

The Green function in the numerator \tilde{G} factorizes into connected and disconnected parts !

$$\begin{aligned} \tilde{G}(x, x'; t - t') &= -i \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \\ &\times \langle \Phi_0 | \hat{T} [\hat{H}_{int}(t_1) \cdots \hat{H}_{int}(t_n) \hat{\Psi}_I(x, t) \hat{\Psi}_I^\dagger(x', t')] | \Phi_0 \rangle_{\text{connected}} \\ &\times \langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle \end{aligned}$$

The closed part of disconnected diagrams

The true Green function:

$$\begin{aligned} G(x, x'; t - t') &= \frac{\tilde{G}(x, x'; t - t')}{\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle} = -i \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \\ &\times \langle \Phi_0 | \hat{T} [\hat{H}_{int}(t_1) \cdots \hat{H}_{int}(t_n) \hat{\Psi}_I(x, t) \hat{\Psi}_I^\dagger(x', t')] | \Phi_0 \rangle_{\text{connected}} \end{aligned}$$

Only connected diagrams need to be taken into account!

The counting factor

For each connected diagram at order n , there are $2^n n!$ Many diagrams that have the same “topological structure”. They differ only in the permutation of the dummy integration variables, and hence yield the same contribution, killing the $1/n!$ prefactor in front (and also 2^n from the Coulomb interaction).

Only topologically different diagrams need to be taken into account!

- For $n=1$, the number of topologically different connected diagrams is 2.
- For $n=2$, this number is 10. (Remember the total number is 120)

The next steps ...

- Dyson equation
- Irreducible self-energy