FIP10601 – Text 13

Green's functions: calculation methods

Equations of motion

One of the usual methods for evaluating Green's functions starts by writing an equation of motion for the desired function. The solution is, in general, approximate.

Let us take, for example, the retarded GF $g^{+}_{\mathbf{k}\sigma}(t)$, introduced in Text 12. Differentiating the equation that defines this time-dependent function [Eq. (1) of Text 12] yields the equation of motion

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} g^{+}_{\mathbf{k}\sigma}(t) &= -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\Big[\theta(t)\langle\{c_{\mathbf{k}\sigma}(t), c^{\dagger}_{\mathbf{k}\sigma}\}\rangle\Big] \\ &= -\mathrm{i}\,\delta(t)\langle\{c_{\mathbf{k}\sigma}, c^{\dagger}_{\mathbf{k}\sigma}\}\rangle - \mathrm{i}\theta(t)\langle\{\dot{c}_{\mathbf{k}\sigma}(t), c^{\dagger}_{\mathbf{k}\sigma}\}\rangle\,, \end{aligned} \tag{1}$$

where $\dot{c}_{\mathbf{k}\sigma}(t)$ denotes the time derivative of $c_{\mathbf{k}\sigma}(t)$, which is given by the Heisenberg equation

$$\dot{c}_{\mathbf{k}\sigma}(t) = -\mathrm{i}\,[c_{\mathbf{k}\sigma}(t), \bar{\mathcal{H}}] \tag{2}$$

(remembering that we are using a unit system in which $\hbar = 1$). Since the anticommutator after $\delta(t)$ in Eq. (1) is known ($= 1$), we can write

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} g^{+}_{\mathbf{k}\sigma}(t) = \delta(t) - \mathrm{i}\theta(t)\langle\{[c_{\mathbf{k}\sigma}(t), \bar{\mathcal{H}}], c^{\dagger}_{\mathbf{k}\sigma}\}\rangle\,. \tag{3}$$

Note that the last term on the r.h.s. is a **new** retarded GF, involving the commutator of $c_{\mathbf{k}\sigma}$ with the Hamiltonian. In most cases this commutator contains products of $c^{\dagger}_{\mathbf{k}\sigma}$ and/or $c_{\mathbf{k}\sigma}$ operators (possibly with other subscripts). This means that the new GF is of *higher order*. When writing the equation of motion for the latter, again a new GF is generated, of even higher order, and so on, giving rise to an *infinite hierarchical chain* of equations of motion.

For a non-interacting system, the commutator $[c_{\mathbf{k}\sigma}(t), \bar{\mathcal{H}}]$ contains a single fermion operator, which is $c_{\mathbf{k}\sigma}(t)$. Then, Eq. (3) is reduced to a single equation for $g^{+}_{\mathbf{k}\sigma}(t)$, whose solution is exact. With interactions, however, one needs to **decouple** a chosen high-order GF in terms of lower-order ones to cut the series. This can be a powerful approximation method to evaluate Green's functions. Its weakness resides in not being systematic, since a specific decoupling is arbitrary, and further corrections cannot be just added in a controlled way.

We will not discuss this method in further detail. We close its presentation remarking that equations of motion for advanced and Matsubara GF's are quite similar to those shown here for the retarded GF, yielding a unified form of the equation of motion in complex-frequency space. This is consistent with these functions being related to one another, as we saw in the discussion of their spectral representations.

Perturbative calculation of the Matsubara GF

In the following, we show that it is possible to formally develop a perturbative method to evaluate the Matsubara GF,

$$\tilde{g}_{\mathbf{k}\sigma}(\tau) \equiv -\langle \hat{T}\, \tilde{c}_{\mathbf{k}\sigma}(\tau) \tilde{c}^{\dagger}_{\mathbf{k}\sigma}(0) \rangle \ , \tag{4}$$

with the time-ordering operator $\hat{T}$, and the τ dependence in the **Heisenberg picture** (with $\bar{\mathcal{H}} = \mathcal{H} - \mu N$), as defined in Text 12. Note that here we introduced a tilde to denote operators with τ dependence in the Heisenberg picture. The reason for this is that in the following we will use the previous notation for operators in the **interaction picture**.

Since the method is not restricted to electrons in solids, and to simplify the notation, we present the perturbative approach for a **generic** fermionic Matsubara GF

$$\tilde{g}_{\alpha\gamma}(\tau) = -\langle \hat{T}\, \tilde{c}_{\alpha}(\tau) \tilde{c}^{\dagger}_{\gamma}(0) \rangle \ , \tag{5}$$

where α and γ represent sets of relevant quantum numbers for the system in question. By definition,

$$\tilde{c}_{\alpha}(\tau) = \mathrm{e}^{\bar{\mathcal{H}}\tau}\, c_{\alpha}\, \mathrm{e}^{-\bar{\mathcal{H}}\tau} \ , \tag{6}$$

and similarly for $\tilde{c}^{\dagger}_{\gamma}(\tau)$.

Initially, we separate the Hamiltonian in two parts,

$$\bar{\mathcal{H}} = \bar{\mathcal{H}}_0 + \mathcal{H}_1 \ , \tag{7}$$

assuming that the eigenvalue problem of $\bar{\mathcal{H}}_0$ is exactly solvable. Choosing the **interaction picture**, the time evolution of operators is given by $\bar{\mathcal{H}}_0$ only. Exemplifying with c_α, we have

$$c_{\alpha}(\tau) = \mathrm{e}^{\bar{\mathcal{H}}_0\tau}\, c_{\alpha}\, \mathrm{e}^{-\bar{\mathcal{H}}_0\tau} \ . \tag{8}$$

We now introduce an operator $S(\tau)$ that relates the Heisenberg and interaction pictures through a similarity transformation of the form

$$c_{\alpha}(\tau) = S(\tau)\, \tilde{c}_{\alpha}(\tau)\, S^{-1}(\tau) \ . \tag{9}$$

Therefore, from Eqs. (6), (8), and (9) we have that

$$S(\tau) = \mathrm{e}^{\bar{\mathcal{H}}_0\tau}\, \mathrm{e}^{-\bar{\mathcal{H}}\tau} \ . \tag{10}$$

With this, the Boltzmann factor appearing in averages may be written as

$$\mathrm{e}^{-\beta\bar{\mathcal{H}}} = \mathrm{e}^{-\beta\bar{\mathcal{H}}_0}\, S(\beta), \tag{11}$$

since β is one of the values of τ. It should be noted that all information about $\mathcal{H}_1$ is contained in $S(\tau)$.

Perturbative calculation of $S(\tau)$

Differentiating Eq. (10) with respect to τ, we have

$$\frac{\mathrm{d}S(\tau)}{\mathrm{d}\tau} = \bar{\mathcal{H}}_0\, \mathrm{e}^{\bar{\mathcal{H}}_0\tau}\, \mathrm{e}^{-\bar{\mathcal{H}}\tau} + \mathrm{e}^{\bar{\mathcal{H}}_0\tau}\, (-\bar{\mathcal{H}})\, \mathrm{e}^{-\bar{\mathcal{H}}\tau} \ . \tag{12}$$

We must be careful **not** to change the order of factors containing $\bar{\mathcal{H}}$ and $\bar{\mathcal{H}}_0$, since these two operators (in general) do not commute.

Equation (12) may be developed as follows.

$$\begin{aligned} \frac{\mathrm{d}S(\tau)}{\mathrm{d}\tau} &= \mathrm{e}^{\bar{\mathcal{H}}_0\tau}\, \bar{\mathcal{H}}_0\, \mathrm{e}^{-\bar{\mathcal{H}}\tau} - \mathrm{e}^{\bar{\mathcal{H}}_0\tau}\, \bar{\mathcal{H}}\, \mathrm{e}^{-\bar{\mathcal{H}}\tau} \\ &= \mathrm{e}^{\bar{\mathcal{H}}_0\tau} (\bar{\mathcal{H}}_0 - \bar{\mathcal{H}})\, \mathrm{e}^{-\bar{\mathcal{H}}\tau} \\ &= -\mathrm{e}^{\bar{\mathcal{H}}_0\tau} \mathcal{H}_1\, \mathrm{e}^{-\bar{\mathcal{H}}\tau} \\ &= -\mathrm{e}^{\bar{\mathcal{H}}_0\tau} \mathcal{H}_1\, \mathrm{e}^{-\bar{\mathcal{H}}_0\tau} \mathrm{e}^{\bar{\mathcal{H}}_0\tau}\, \mathrm{e}^{-\bar{\mathcal{H}}\tau} \ . \end{aligned} \tag{13}$$

This yields the equation of motion

$$\frac{\mathrm{d}S(\tau)}{\mathrm{d}\tau} = -\mathcal{H}_1(\tau) S(\tau) \ , \tag{14}$$

where $\mathcal{H}_1(\tau)$ has its τ dependence in the interaction picture.

***Formal* solution of the equation of motion for $S(\tau)$**

If we **were** dealing with commuting functions, Eq. (12) **would** have the solution

$$S(\tau) = \exp\left[-\int_0^\tau \mathrm{d}\tau'\, \mathcal{H}_1(\tau') \right] \ . \tag{15}$$

However, given that $\bar{\mathcal{H}}_0$ and $\mathcal{H}_1$ do not commute, the operators $\mathcal{H}_1(\tau)$ and $\mathcal{H}_1(\tau')$ at different times do not commute either. Then, remembering that the exponential function (like any function of an operator) should be interpreted as the sum of its power series, we must keep the products of $\mathcal{H}_1$'s **ordered** in τ in each term of the series. Therefore, the solution to Eq. (14) involves the time-ordering operator, and may be written in the form

$$S(\tau) = \hat{T}\, \exp\left[-\int_0^\tau \mathrm{d}\tau'\, \mathcal{H}_1(\tau') \right] \ , \tag{16}$$

which is to be interpreted as

$$S(\tau) = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \int_0^\tau \mathrm{d}\tau_1 \ldots \int_0^\tau \mathrm{d}\tau_n\, \hat{T}\, \mathcal{H}_1(\tau_1) \ldots \mathcal{H}_1(\tau_n) \ . \tag{17}$$

Perturbative expansion of the Green's function

Starting with the definition of the Matsubara GF, Eq. (5), and using Eqs. (9) and (11), we have

$$\begin{aligned}\tilde{g}_{\alpha\gamma}(\tau) &= -\langle \hat{T}\, \tilde{c}_\alpha(\tau)\tilde{c}^\dagger_\gamma(0)\rangle \\ &= -\frac{\mathrm{Tr}\, \mathrm{e}^{-\beta\bar{\mathcal{H}}}\, \hat{T} S^{-1}(\tau)\, c_\alpha(\tau)\, S(\tau) c^\dagger_\gamma(0)}{\mathrm{Tr}\, \mathrm{e}^{-\beta\bar{\mathcal{H}}}} \\ &= -\frac{\mathrm{Tr}\, \mathrm{e}^{-\beta\bar{\mathcal{H}}_0} S(\beta)\, \hat{T} S^{-1}(\tau)\, c_\alpha(\tau)\, S(\tau) c^\dagger_\gamma(0)}{\mathrm{Tr}\, \mathrm{e}^{-\beta\bar{\mathcal{H}}_0} S(\beta)}\,. \end{aligned} \tag{18}$$

Now, we should observe that:

- **Inside** the time-ordered product (i.e., under the action of $\hat{T}$), the positions of $S(\tau)$ and $c_\alpha(\tau)$ may be exchanged, since the former contains an even number of fermion operators, which implies that there is no sign change. This causes the factors $S(\tau)$ and $S^{-1}(\tau)$ to cancel out.
- Since the operator $S(\beta)$ is positioned to the left of the time-ordering operator but its time is the highest possible, it may be placed **anywhere inside** the time-ordered product.

So, we can write

$$\tilde{g}_{\alpha\gamma}(\tau) = -\frac{\langle \hat{T}\, c_\alpha(\tau) c^\dagger_\gamma(0) S(\beta)\rangle_0}{\langle S(\beta)\rangle_0}\,, \tag{19}$$

or, using Eq. (17),

$$\tilde{g}_{\alpha\gamma}(\tau) = -\frac{\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_n \langle \hat{T}\, c_\alpha(\tau) c^\dagger_\gamma(0) \mathcal{H}_1(\tau_1)\ldots\mathcal{H}_1(\tau_n)\rangle_0}{\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_n \langle \hat{T}\, \mathcal{H}_1(\tau_1)\ldots\mathcal{H}_1(\tau_n)\rangle_0}\,. \tag{20}$$

The subscript *zero* on the averages reflects the fact that the Boltzmann factor contains only $\mathcal{H}_0$.

Application to the electronic GF

We now apply the generic perturbative formalism just developed to the GF that describes single-electron excitations in a metal.

First, let us remember the form of the Hamiltonian (keeping the e-e interaction term as obtained for the homogeneous case),

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\substack{\mathbf{k}\mathbf{k}'\mathbf{q} \\ \sigma\sigma'}} U(\mathbf{q})\; c^\dagger_{\mathbf{k}+\mathbf{q},\sigma}\, c^\dagger_{\mathbf{k}'-\mathbf{q},\sigma'}\, c_{\mathbf{k}'\sigma'}\, c_{\mathbf{k}\sigma}\,. \tag{21}$$

We choose the band term as $\bar{\mathcal{H}}_0$ and the e-e interaction part as $\mathcal{H}_1$.

At this point, the alert student remembers our previous conclusion that the interaction term cannot be treated as a perturbation. It is true, and we must state clearly what will be done. We cannot just evaluate a few terms of the perturbation series and neglect the subsequent ones. We will use a method that allows to sum **infinite series**, that is, to take into account contributions to **all orders** (though not the full contribution of each order).

We want to evaluate

$$\tilde{g}_{\mathbf{k}\sigma}(\tau) = -\langle \hat{T}\, \tilde{c}_{\mathbf{k}\sigma}(\tau)\tilde{c}^{\dagger}_{\mathbf{k}\sigma}(0)\rangle = -\frac{\langle \hat{T}\, c_{\mathbf{k}\sigma}(\tau)c^{\dagger}_{\mathbf{k}\sigma}(0)S(\beta)\rangle_0}{\langle S(\beta)\rangle_0}\ , \tag{22}$$

which, from Eq. (20), becomes

$$\tilde{g}_{\mathbf{k}\sigma}(\tau) = -\frac{\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_n \langle \hat{T}\, c_{\mathbf{k}\sigma}(\tau)c^{\dagger}_{\mathbf{k}\sigma}(0)\mathcal{H}_1(\tau_1)\ldots\mathcal{H}_1(\tau_n)\rangle_0}{\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_n \langle \hat{T}\, \mathcal{H}_1(\tau_1)\ldots\mathcal{H}_1(\tau_n)\rangle_0}\ . \tag{23}$$

Wick's theorem

From the form of $\mathcal{H}_1$, we see that the averages in Eq. (23) involve products of creation and annihilation operators (in equal number), each operator associated to some "time". For M operators of each type, we have an *M-particle propagator*. Given that the average refers to a non-interacting system, these M particles propagate **independently**. This means that the average **decouples** into M **single-particle** GF's, summed over all possible decouplings, i.e., all forms of dividing the $2M$ original operators in M creation-annihilation pairs. Such a decoupling scheme can be rigorously demonstrated, and constitutes the so-called *Wick's Theorem*. We will not develop the demonstration here, as this would lead to a more detailed discussion of technical aspects than necessary to our purposes.

Zeroth order GF

Considering that Wick's theorem leads to decoupling all averages into products of zeroth-order GF's, we begin by solving the non-interacting problem, which can be done exactly.

From the definition of the Matsubara GF, we have

$$\begin{aligned}\tilde{g}^0_{\mathbf{k}\sigma}(\tau) &= -\langle \hat{T}\, c_{\mathbf{k}\sigma}(\tau)c^{\dagger}_{\mathbf{k}\sigma}(0)\rangle_0 \\ &= -\theta(\tau)\langle c_{\mathbf{k}\sigma}(\tau)c^{\dagger}_{\mathbf{k}\sigma}(0)\rangle_0 + \theta(-\tau)\langle c^{\dagger}_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(\tau)\rangle_0\ .\end{aligned} \tag{24}$$

Using the explicit form of the non-interacting Hamiltonian, we can show **(EXERCISE)** that

$$c_{\mathbf{k}\sigma}(\tau) = \mathrm{e}^{-\bar{\varepsilon}_{\mathbf{k}}\tau}c_{\mathbf{k}\sigma}\ . \tag{25}$$

Then,

$$\begin{aligned}\tilde{g}^0_{\mathbf{k}\sigma}(\tau) &= \mathrm{e}^{-\bar{\varepsilon}_{\mathbf{k}}\tau}\left[\theta(-\tau)\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle_0 - \theta(\tau)\langle c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}\rangle_0\right] \\ &= \mathrm{e}^{-\bar{\varepsilon}_{\mathbf{k}}\tau}\Big\{\theta(-\tau)f(\varepsilon_{\mathbf{k}}) - \theta(\tau)[1-f(\varepsilon_{\mathbf{k}})]\Big\}\,, \end{aligned} \tag{26}$$

where $f(\varepsilon)$ is the Fermi function. Note that the zeroth-order GF does not depend on spin, but we keep the σ index to indicate that the electron is in a well-defined spin state.

Taking the Fourier transform

$$\begin{aligned}\tilde{G}^0_{\mathbf{k}\sigma}(\omega_n) &= \int_0^\beta \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\tilde{g}_{\mathbf{k}\sigma}(\tau) \\ &= -[1-f(\varepsilon_{\mathbf{k}})]\int_0^\beta \mathrm{d}\tau\, \mathrm{e}^{(\mathrm{i}\omega_n-\bar{\varepsilon}_{\mathbf{k}})\tau}\,, \end{aligned} \tag{27}$$

and after a simple algebraic development, we arrive at

$$\tilde{G}^0_{\mathbf{k}\sigma}(\omega_n) = \frac{1}{\mathrm{i}\omega_n - \varepsilon_{\mathbf{k}} + \mu}\,\cdot \tag{28}$$

Here we can explicitly verify the general properties of GF's. Analytic continuation to real frequencies yields the retarded GF

$$G^{0+}_{\mathbf{k}\sigma}(\omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}} + \mu + \mathrm{i}\eta}\,\cdot \tag{29}$$

This function is analytic except for poles whose real parts are at frequencies $\omega = \varepsilon_{\mathbf{k}} - \mu$. These are the single-particle *excitation energies* in the non-interacting case, which are just individual electron energies measured from the chemical potential. The density of states for these excitations is

$$\rho_\sigma(\omega) = -\frac{1}{\pi N}\sum_{\mathbf{k}} \mathrm{Im}\, G^{0+}_{\mathbf{k}\sigma}(\omega) = \frac{1}{N}\sum_{\mathbf{k}} \delta(\omega - \varepsilon_{\mathbf{k}} + \mu)\,. \tag{30}$$

Except for the displacement of the frequency range, which has $\omega = 0$ corresponding to $\varepsilon_{\mathbf{k}} = \mu$, we recognize the general definition of density of states for independent electrons.

Now, once we know the zeroth-order GF, the perturbative calculation can be worked out starting from Eq. (23). A systematization of this procedure is presented below.

Diagrammatic representation

As a result of Wick's theorem applied to Eq. (23), the terms of the GF perturbation series (both numerator and denominator) contain products of factors $U(\mathbf{q})$ and zeroth-order GF's, which are integrated over *internal* τ's, summed over *internal* wavevectors, and summed

over *internal* spin states. But the number of such terms may be large, and quickly increases at higher orders of perturbation. On the other hand, many terms are seen to be equivalent by changes of integration or summation variables.

To facilitate a systematization of the method, a **diagrammatic representation** (Feynman diagrams) is usually employed, with the zeroth-order GF and $U(\mathbf{q})$ represented as follows:

$\tilde{g}^0_{\mathbf{k}\sigma}(\tau)$: 

$U(\mathbf{q})$: (31)

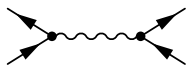
The *beginning* of a $\tilde{g}^0$ line is the time associated to the creation operator, while its *end* time is the one associated to the annihilation operator.

The two extreme points of an interaction line are each associated to a **pair** of creation and annihilation operators, being therefore points where a $\tilde{g}^0$ line ends and another one begins.

The points of a diagram that are beginning, end, or connection of lines are called *vertices*.

Then the *basic ingredients* of the diagrammatic representation of a Matsubara GF are:

 : two *external* vertices, associated to the operators that define the GF;

 : an interaction line for each $\mathcal{H}_1$, connecting *internal* vertices.

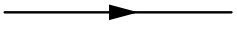
With these ingredients, the application of Wick's theorem consists in connecting the vertices through $\tilde{g}^0$ lines in every possible way, thus constructing several **diagrams** that represent the terms in each order of perturbation. At a given order n, there are n interaction lines, hence $2n$ internal vertices and two external ones. In each diagram, there is wavevector conservation at each internal vertex, whereas the external wavevector $\mathbf{k}$ *enters* the diagram at the initial vertex (time *zero*) and *exits* at the end vertex (time τ).

After writing the corresponding expressions, the contributions of all diagrams (in principle, of all orders!) are just added.

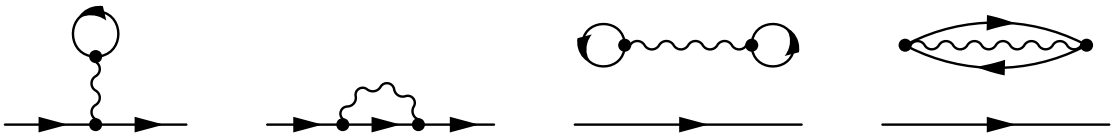
It should be noted that there is a sum of diagrams associated with the numerator and another to the denominator of Eq. (23). Only the diagrams representing the numerator contain external vertices.

To arrive at the final form of the diagrammatic representation, let us analyze some examples of numerator diagrams.

The only zeroth-order diagram is obviously a single $\tilde{g}^0$ line:



The first order diagrams are shown below.



The last two diagrams are **disconnected**. This kind of diagram is always composed by a *connected* part, which (by definition) includes the two external vertices, and one or more *disconnected* parts, which contain only **internal** vertices.

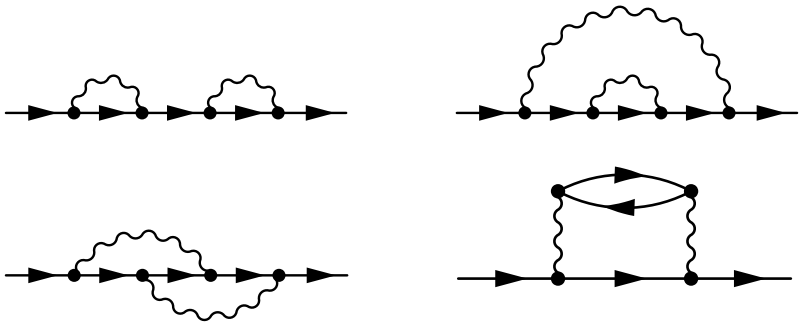
Extending to higher orders, and taking into account that each diagram corresponds to a well-defined mathematical expression, it is not difficult to see that the sum of numerator diagrams can be viewed as a product of two factors. One factor is the sum of all connected parts, and the other is the unity plus the sum of all disconnected parts. But diagrams with only internal vertices are the ones that constitute the diagrammatic representation of the **denominator** of Eq. (22), whose expansion up to first order, as can be inferred from the explicit form in Eq. (23), is given by

$$\langle S(\beta)\rangle_0 = 1 + \quad + \quad + \cdots \tag{32}$$

Therefore, the second factor in the numerator (containing only internal parts) **exactly cancels** the denominator. The final result is that the GF is just given by the sum of all **fully connected** diagrams.

For the homogeneous system that we are considering, diagrams that contain a $\tilde{g}^0$ line closed in itself are **null**, as they contain an interaction line with $q = 0$. So, the diagrams that effectively contribute up to second order are shown below.

- Zeroth order:
- First order: 
- Second order:

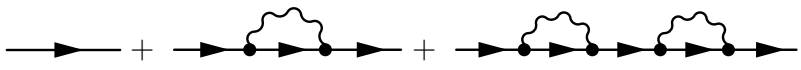


It is usual (and convenient) to take the "time" Fourier transform, generating a frequency-dependent GF. There is no change in the diagrammatic representation. However,

- lines now represent $\tilde{G}^0$'s dependent on Matsubara frequencies;
- instead of integrals over internal τ's we have sums over internal Matsubara frequencies (each sum with a factor $1/\beta$);
- vertices no longer correspond to specific times, but there is *frequency conservation* at each internal vertex, while the external frequency ω_n enters a diagram at the initial vertex and exits at the end one.

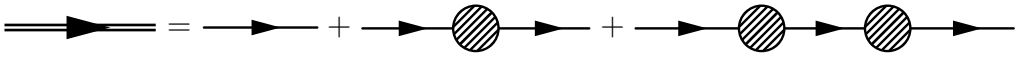
Sums of infinite series

From the diagrams up to order two, we can select, for example, the following series:



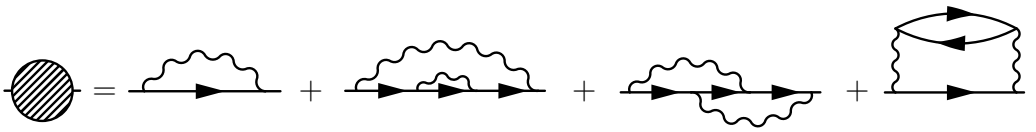
(33)

This particular series exemplifies the general structure of the GF diagrammatic expansion, which can be schematically depicted as



(34)

The dark circle represents the so-called **self-energy**, denoted by $\Sigma_{\mathbf{k}\sigma}(\omega_n)$. It is the sum of all **irreducible internal parts**. *Internal* means that the part does not include either the initial or the final $\tilde{G}^0$ line. *Irreducible* means that it cannot be divided into two disconnected parts by cutting a single $\tilde{G}^0$ line. From the diagrams up to order two, we have



(35)

and so on to higher orders, with self-energy parts containing more interaction lines.

The diagrammatic series (34) can be translated into the equation

$$\begin{aligned}\tilde{G}_{\mathbf{k}\sigma}(\omega_n) &= \tilde{G}^0_{\mathbf{k}\sigma}(\omega_n) + \tilde{G}^0_{\mathbf{k}\sigma}(\omega_n)\Sigma_{\mathbf{k}\sigma}(\omega_n)\tilde{G}^0_{\mathbf{k}\sigma}(\omega_n) \\ &\quad + \tilde{G}^0_{\mathbf{k}\sigma}(\omega_n)\Sigma_{\mathbf{k}\sigma}(\omega_n)\tilde{G}^0_{\mathbf{k}\sigma}(\omega_n)\Sigma_{\mathbf{k}\sigma}(\omega_n)\tilde{G}^0_{\mathbf{k}\sigma}(\omega_n) + \ldots \end{aligned} \tag{36}$$

Using a simplified notation, and reorganizing the above equation as

$$G = G^0 + G^0\Sigma\,[G^0 + G^0\Sigma\,G^0 + G^0\Sigma\,G^0\Sigma\,G^0 + \ldots]\,, \tag{37}$$

we see that

$$G = G^0 + G^0\Sigma\,G\,. \tag{38}$$

The last equality has a structure known as *Dyson's equation*. Its *formal* solution is

$$G = \frac{G^0}{1 - G^0\Sigma} = \frac{1}{(G^0)^{-1} - \Sigma}\,. \tag{39}$$

Going back to full notation, and remembering that $[\tilde{G}^0_{\mathbf{k}\sigma}(\omega_n)]^{-1} = \mathrm{i}\omega_n - \varepsilon_{\mathbf{k}} + \mu$, we arrive at the final **formal solution**

$$\tilde{G}_{\mathbf{k}\sigma}(\omega_n) = \frac{1}{\mathrm{i}\omega_n - \varepsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}\sigma}(\omega_n) + \mu}\,. \tag{40}$$

The problem is therefore "reduced" to evaluate the self-energy. Note that any approximation for Σ (finite number of diagrams) corresponds to an **infinite series** for the GF.

In the next Text we will explore the above formal solution to deduce general properties of single-particle excitations in the interacting electron system.