FIP10601 – Text 12

Green's-function approach to interacting electrons

In the beginning of our discussion of electron-electron interaction in solids we remarked that the concept of *individual* energies is not applicable to systems of many interacting particles. Afterwards, we have seen that evaluation of the *total* energy is essentially restricted to the ground state in usual approximation methods. From the point of view of comparison with experimental results, it is actually more relevant to describe *elementary excitations*. We already mentioned that the energy spectrum of *single-particle excitations* is of special interest because of its connection with individual energies in the non-interacting limit. Such excitations are best described by means of *Green's functions*, which we now begin to study.

One-particle Green's function

Two versions of a single-particle Green's function (GF) for the specific problem of interacting electrons in the conduction band of a metallic solid are defined as

$$g^{\pm}_{\mathbf{k}\sigma}(t) \equiv \mp \mathrm{i}\theta(\pm t)\langle\{c_{\mathbf{k}\sigma}(t), c^{\dagger}_{\mathbf{k}\sigma}(0)\}\rangle \; . \tag{1}$$

The + and − superscripts indicate respectively *retarded* ($t > 0$) and *advanced* ($t < 0$) GF's, chosen through the step functions $\theta(\pm t)$. This definition involves an *anticommutator* of annihilation an creation operators, which is the appropriate choice for fermions (an equivalent definition for bosons would involve the *commutator*). We work in the *Heisenberg picture* (or *Heisenberg representation*), so that operators are time dependent. A few comments are in order concerning Eq. (1).

- Choosing the first operator at time t and the second at time 0 (zero) is **not** restrictive. It can be easily shown that it is equivalent to having the creation operator at a time t' and the annihilation operator at a time t'' such that $t'' - t' = t$.
- We are interested in finite temperatures. Therefore, the mean value must be interpreted as a quantum statistical average. Since we are dealing with operators that change the number of particles, we must use the *gran-canonical* ensemble. So, the average is defined as

  $$\langle X\rangle = Z^{-1}\mathrm{Tr}\,\mathrm{e}^{-\beta\bar{\mathcal{H}}}X \; , \quad Z = \mathrm{Tr}\,\mathrm{e}^{-\beta\bar{\mathcal{H}}} \; , \tag{2}$$

  where

  $$\beta \equiv 1/T \; , \qquad \bar{\mathcal{H}} \equiv \mathcal{H} - \mu N \; , \tag{3}$$

  T being the temperature, μ the chemical potential, $\mathcal{H}$ the Hamiltonian, and N the total-number **operator**.

- We will see that it is convenient to redefine the *Heisenberg picture* to use the "Hamiltonian" $\bar{\mathcal{H}}$ defined in Eq. (3), i.e.,

$$A(t) \equiv \mathrm{e}^{\mathrm{i}\bar{\mathcal{H}}t} A \, \mathrm{e}^{-\mathrm{i}\bar{\mathcal{H}}t} \; . \tag{4}$$

  This modification does not affect the time evolution of any operator that conserves the number of particles (as, for instance, the Hamiltonian).

- We omitted k_B in the definition of β, and $1/\hbar$ in the exponents of Eq. (4). This is equivalent to adopting a "units system" in which $k_B = \hbar = 1$ (implying that energy, frequency, and temperature have the same unit).

Next we demonstrate that the GF's defined in Eq. (1) allow to obtain the energy spectrum of single-particle excitations.

Expanding the anticommutator in the r.h.s. of Eq. (1), we have

$$g^{\pm}_{\mathbf{k}\sigma}(t) \equiv \mp \mathrm{i}\theta(\pm t) \left\{ \langle c_{\mathbf{k}\sigma}(t) c^{\dagger}_{\mathbf{k}\sigma}(0) \rangle + \langle c^{\dagger}_{\mathbf{k}\sigma}(0) c_{\mathbf{k}\sigma}(t) \rangle \right\} \; . \tag{5}$$

We will **formally** evaluate average values in the energy representation, that is, using the (supposedly existing) solutions of the eigenvalue problem

$$\bar{\mathcal{H}}|n\rangle = \bar{E}_n |n\rangle \; , \qquad \bar{E}_n \equiv E_n - \mu N \; , \tag{6}$$

with the eigenvectors obeying the relationships

$$\langle n|m\rangle = \delta_{nm} \; , \qquad \sum_n |n\rangle\langle n| = 1 \; . \tag{7}$$

Note that $|n\rangle$ represents, in compact notation, an energy eigenstate of the **entire system of interacting electrons**, which can be written as a linear combination of Fock-space basis vectors in the occupation-number representation, $|n_{\mathbf{k}_1\sigma_1} \, n_{\mathbf{k}_2\sigma_2} \, n_{\mathbf{k}_3\sigma_3} \, \ldots\rangle$.

Let us develop the first average on the r.h.s. of Eq. (5) as follows.

$$\begin{aligned}
\langle c_{\mathbf{k}\sigma}(t) c^{\dagger}_{\mathbf{k}\sigma}(0) \rangle &= Z^{-1} \mathrm{Tr} \, \mathrm{e}^{-\beta\bar{\mathcal{H}}} \mathrm{e}^{\mathrm{i}\bar{\mathcal{H}}t} c_{\mathbf{k}\sigma} \mathrm{e}^{-\mathrm{i}\bar{\mathcal{H}}t} c^{\dagger}_{\mathbf{k}\sigma} \\
&= Z^{-1} \sum_n \langle n| \mathrm{e}^{-\beta\bar{\mathcal{H}}} \mathrm{e}^{\mathrm{i}\bar{\mathcal{H}}t} c_{\mathbf{k}\sigma} \mathrm{e}^{-\mathrm{i}\bar{\mathcal{H}}t} c^{\dagger}_{\mathbf{k}\sigma} |n\rangle \\
&= Z^{-1} \sum_{nm} \langle n| \mathrm{e}^{-\beta\bar{\mathcal{H}}} \mathrm{e}^{\mathrm{i}\bar{\mathcal{H}}t} c_{\mathbf{k}\sigma} \mathrm{e}^{-\mathrm{i}\bar{\mathcal{H}}t} |m\rangle\langle m| c^{\dagger}_{\mathbf{k}\sigma} |n\rangle \\
&= Z^{-1} \sum_{nm} \mathrm{e}^{-\beta\bar{E}_n} \mathrm{e}^{\mathrm{i}(\bar{E}_n - \bar{E}_m)t} \langle n| c_{\mathbf{k}\sigma} |m\rangle\langle m| c^{\dagger}_{\mathbf{k}\sigma} |n\rangle \; .
\end{aligned} \tag{8}$$

Similarly, for the second average,

$$\begin{aligned}
\langle c^{\dagger}_{\mathbf{k}\sigma}(0) c_{\mathbf{k}\sigma}(t) \rangle &= Z^{-1} \mathrm{Tr} \, \mathrm{e}^{-\beta\bar{\mathcal{H}}} c^{\dagger}_{\mathbf{k}\sigma} \mathrm{e}^{\mathrm{i}\bar{\mathcal{H}}t} c_{\mathbf{k}\sigma} \mathrm{e}^{-\mathrm{i}\bar{\mathcal{H}}t} \\
&= Z^{-1} \sum_m \langle m| \mathrm{e}^{-\beta\bar{\mathcal{H}}} c^{\dagger}_{\mathbf{k}\sigma} \mathrm{e}^{\mathrm{i}\bar{\mathcal{H}}t} c_{\mathbf{k}\sigma} \mathrm{e}^{-\mathrm{i}\bar{\mathcal{H}}t} |m\rangle \\
&= Z^{-1} \sum_{nm} \langle m| \mathrm{e}^{-\beta\bar{\mathcal{H}}} c^{\dagger}_{\mathbf{k}\sigma} |n\rangle\langle n| \mathrm{e}^{\mathrm{i}\bar{\mathcal{H}}t} c^{\dagger}_{\mathbf{k}\sigma} \mathrm{e}^{-\mathrm{i}\bar{\mathcal{H}}t} |m\rangle \\
&= Z^{-1} \sum_{nm} \mathrm{e}^{-\beta\bar{E}_m} \mathrm{e}^{\mathrm{i}(\bar{E}_n - \bar{E}_m)t} \langle m| c^{\dagger}_{\mathbf{k}\sigma} |n\rangle\langle n| c_{\mathbf{k}\sigma} |m\rangle \; .
\end{aligned} \tag{9}$$

Therefore,

$$g^{\pm}_{\mathbf{k}\sigma}(t) = \mp \mathrm{i}\,\theta(\pm t) Z^{-1} \sum_{nm} \left(\mathrm{e}^{-\beta \bar{E}_n} + \mathrm{e}^{-\beta \bar{E}_m} \right) \langle n | c_{\mathbf{k}\sigma} | m \rangle \langle m | c^{\dagger}_{\mathbf{k}\sigma} | n \rangle \mathrm{e}^{\mathrm{i}(\bar{E}_n - \bar{E}_m)t} \; . \tag{10}$$

Defining frequency-dependent GF's as the Fourier transforms of $g^{\pm}_{\mathbf{k}\sigma}(t)$,

$$G^{\pm}_{\mathbf{k}\sigma}(\omega) \equiv \int_{-\infty}^{\infty} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}\omega t} g^{\pm}_{\mathbf{k}\sigma}(t) \; , \tag{11}$$

we have

$$G^{\pm}_{\mathbf{k}\sigma}(\omega) = \mp \mathrm{i}\, Z^{-1} \sum_{nm} \left(\mathrm{e}^{-\beta \bar{E}_n} + \mathrm{e}^{-\beta \bar{E}_m} \right) \langle n | c_{\mathbf{k}\sigma} | m \rangle \langle m | c^{\dagger}_{\mathbf{k}\sigma} | n \rangle \int_{-\infty}^{\infty} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}\,[\omega - (\bar{E}_m - \bar{E}_n)]t} \theta(\pm t)] \; . \tag{12}$$

Using the identity

$$\int_{-\infty}^{\infty} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}\alpha t} \theta(\pm t) = \lim_{\eta \to 0} \frac{\mp 1}{\mathrm{i}\,(\alpha \pm \mathrm{i}\eta)} \; , \tag{13}$$

and (from now on) **implicitly** assuming the limit $\eta \to 0$, we obtain

$$G^{\pm}_{\mathbf{k}\sigma}(\omega) = Z^{-1} \sum_{nm} \left(\mathrm{e}^{-\beta \bar{E}_n} + \mathrm{e}^{-\beta \bar{E}_m} \right) \frac{\langle n | c_{\mathbf{k}\sigma} | m \rangle \langle m | c^{\dagger}_{\mathbf{k}\sigma} | n \rangle}{\omega - (\bar{E}_m - \bar{E}_n) \pm \mathrm{i}\eta} \; . \tag{14}$$

Inspecting the r.h.s. of this last equation we observe that the Green's functions $G^{\pm}_{\mathbf{k}\sigma}(\omega)$ are analytic functions of ω except for poles immediately below (retarded GF) or above (advanced GF) the real axis on the **complex**-frequency plane. The real part of each pole is a frequency corresponding to the energy difference between two states whose numbers of particles differ by ± 1. If we assume that the state $|n\rangle$ corresponds to N particles, the matrix element $\langle m | c^{\dagger}_{\mathbf{k}\sigma} | n \rangle$ is nonzero only if $|m\rangle$ corresponds to $(N+1)$ particles. Then,

$$\bar{E}_m - \bar{E}_n = E^{(N+1)}_m - \mu(N+1) - E^{(N)}_n + \mu N = E^{(N+1)}_m - E^{(N)}_n - \mu \; . \tag{15}$$

This is an excitation energy due to creation of an extra particle. Equation (5), and therefore Eq. (14), include the possibility of first creating a particle and later annihilating it (illustrated in the last equation), as well as the possibility of first annihilating a particle and later creating one, then involving states with N and $N-1$ particles. This latter "process" can be viewed as the creation (and subsequent annihilation) of a *hole*. Considering both possibilities, these poles provide the single-particle excitation spectrum.

Isolated particle (or hole) excitations, as described by the GF's introduced here, can occur only by adding a particle to the system (or subtracting one from it), thus involving an external source. On the other hand, it is possible to have a pair of excitations, one of each kind, conserving the number of particles. Later on we will see that such *particle-hole* excitations are the lowest-energy elementary excitations in a metal.

Spectral representation

It is possible express the retarded and advanced GF's in a simple integral form,

$$G^{\pm}_{\mathbf{k}\sigma}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \frac{\rho_{\mathbf{k}\sigma}(\varepsilon)}{\omega - \varepsilon \pm \mathrm{i}\eta} \,, \tag{16}$$

usually called *spectral representation*, by defining the *spectral function*

$$\rho_{\mathbf{k}\sigma}(\varepsilon) \equiv Z^{-1} \sum_{nm} \left(\mathrm{e}^{-\beta \bar{E}_n} + \mathrm{e}^{-\beta \bar{E}_m} \right) \langle n | c_{\mathbf{k}\sigma} | m \rangle \langle m | c^{\dagger}_{\mathbf{k}\sigma} | n \rangle \, \delta(\varepsilon - \bar{E}_m + \bar{E}_n) \,. \tag{17}$$

The quantity

$$\rho_{\sigma}(\varepsilon) \equiv \frac{1}{N} \sum_{\mathbf{k}} \rho_{\mathbf{k}\sigma}(\varepsilon) \tag{18}$$

can be viewed as a generalization of the density of states (DOS), previously introduced for independent electrons. Here it is actually the density of possible energies of single-particle excitations. In the noninteracting limit these energies are those of available single-electron states, and the independent-electron DOS is recovered.

Separating real and imaginary parts in Eq. (16), and using the identity

$$\lim_{\eta \to 0} \frac{1}{\pi} \frac{\eta}{x^2 + \eta^2} = \delta(x) \,, \tag{19}$$

we see that

$$\rho_{\mathbf{k}\sigma}(\omega) = \mp \frac{1}{\pi} \mathrm{Im}\, G^{\pm}_{\mathbf{k}\sigma}(\omega) \,. \tag{20}$$

This relationship is very important because the formal definition (17) cannot be used in practice to evaluate the spectral density, as it would involve solving the eigenvalue problem of a many-body Hamiltonian. On the other hand, as we will see later, approximation methods can be devised to directly evaluate Green's functions. Then, the spectral density given by Eq. (20) allows to obtain the DOS through Eq. (18).

Causal GF

One can also define a GF that coincides with the retarded one for $t > 0$, and with the advanced one for $t < 0$. This is the *causal Green's function*,

$$g^{c}_{\mathbf{k}\sigma}(t) \equiv -\mathrm{i} \langle \hat{T} c_{\mathbf{k}\sigma}(t) c^{\dagger}_{\mathbf{k}\sigma}(0) \rangle \,, \tag{21}$$

involving the **time-ordering operator** $\hat{T}$, which is actually a "super operator" since it acts on operators. Its action on a generic product of operators A and B is defined as

$$\hat{T} A(t) B(t') \equiv A(t) B(t') \theta(t - t') \pm B(t') A(t) \theta(t' - t) \,, \tag{22}$$

with the upper(lower) sign applying to bosons(fermions).

Through the same kind of development utilized above for retarded and advanced GF's, we obtain that the causal GF has a spectral representation of the form

$$G^c_{\mathbf{k}\sigma}(\omega) = \int_0^\infty \mathrm{d}\varepsilon \left[\frac{A_{\mathbf{k}\sigma}(\varepsilon)}{\omega - \varepsilon + \mathrm{i}\eta} + \frac{B_{\mathbf{k}\sigma}(\varepsilon)}{\omega + \varepsilon - \mathrm{i}\eta} \right] , \tag{23}$$

where

$$\begin{aligned} A_{\mathbf{k}\sigma}(\varepsilon) &\equiv Z^{-1} \sum_{nm} \mathrm{e}^{-\beta \bar{E}_n} \langle n|c_{\mathbf{k}\sigma}|m\rangle \langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle \, \delta(\varepsilon - \bar{E}_m + \bar{E}_n) , \\ B_{\mathbf{k}\sigma}(\varepsilon) &\equiv Z^{-1} \sum_{nm} \mathrm{e}^{-\beta \bar{E}_n} \langle n|c^\dagger_{\mathbf{k}\sigma}|m\rangle \langle m|c_{\mathbf{k}\sigma}|n\rangle \, \delta(\varepsilon + \bar{E}_m - \bar{E}_n) . \end{aligned} \tag{24}$$

This spectral representation has two parts: a retarded one, corresponding to particle excitations, and an advanced one, corresponding to hole excitations.

Here we see an interesting identification of particle propagation **back in time** with forward propagation of a hole. This is an appealing feature of the causal GF. On the other hand, the two terms in Eq. (23) are not convenient if we seek a DOS, for which a spectral representation like Eq. (16) is appropriate. In both cases, there is also the need to deal with time and temperature appearing in real and complex exponential functions of the Hamiltonian. Fortunately, all these issues can be dealt with in a clever way, described in the following section.

Matsubara GF

To avoid mixing real and complex exponential functions when evaluating GF's at finite temperature, Matsubara introduced a modified causal GF, defined by

$$\tilde{g}_{\mathbf{k}\sigma}(\tau) \equiv -\langle \hat{T}\, c_{\mathbf{k}\sigma}(\tau) c^\dagger_{\mathbf{k}\sigma}(0) \rangle , \tag{25}$$

where the "time" dependence of operators is redefined to be

$$A(\tau) \equiv \mathrm{e}^{\bar{\mathcal{H}}\tau} A \, \mathrm{e}^{-\bar{\mathcal{H}}\tau} . \tag{26}$$

Although τ is a real variable, it is referred to as *imaginary time* since it replaces the product $\mathrm{i}t$ in the usual Heisenberg picture. By definition, τ in Eq. (26) is continuous in the finite range $[0, \beta]$. This restriction, as we will see, allows β-dependent exponentials associated to ensemble averages to find a "natural" position within the τ-ordering. We keep the same notation for the time-ordering operator $\hat{T}$, and its definition remains the same (with the replacement $t \to \tau$).

It should be noticed that τ as it appears in Eq. (25) is defined in the range $[-\beta, \beta]$ since it is actually a difference of two τ's. This apparent source of ambiguity disappears when one resorts to Fourier representation, as we will see next.

Spectral representation for the Matsubara GF

The fact that τ is defined in a finite range implies that we must use Fourier series instead of Fourier transforms.

Initially, we will determine an important property of $\tilde{g}_{\mathbf{k}\sigma}(\tau)$ that will define the relevant range for evaluating its Fourier components. Explicitly applying the τ-ordering in Eq. (25), we have

$$\tilde{g}_{\mathbf{k}\sigma}(\tau) = -\theta(\tau)\langle c_{\mathbf{k}\sigma}(\tau)c^{\dagger}_{\mathbf{k}\sigma}(0)\rangle + \theta(-\tau)\langle c^{\dagger}_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(\tau)\rangle \; . \tag{27}$$

Developing the second average as follows,

$$\begin{aligned}
\langle c^{\dagger}_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(\tau)\rangle &= Z^{-1}\mathrm{Tr}\, \mathrm{e}^{-\beta\bar{\mathcal{H}}}c^{\dagger}_{\mathbf{k}\sigma}\mathrm{e}^{\bar{\mathcal{H}}\tau}c_{\mathbf{k}\sigma}\mathrm{e}^{-\bar{\mathcal{H}}\tau} \\
&= Z^{-1}\mathrm{Tr}\, \mathrm{e}^{\bar{\mathcal{H}}\tau}c_{\mathbf{k}\sigma}\mathrm{e}^{-\bar{\mathcal{H}}\tau}\mathrm{e}^{-\beta\bar{\mathcal{H}}}c^{\dagger}_{\mathbf{k}\sigma} \\
&= Z^{-1}\mathrm{Tr}\, \mathrm{e}^{-\beta\bar{\mathcal{H}}}\mathrm{e}^{\beta\bar{\mathcal{H}}}\mathrm{e}^{\bar{\mathcal{H}}\tau}c_{\mathbf{k}\sigma}\mathrm{e}^{-\bar{\mathcal{H}}\tau}\mathrm{e}^{-\beta\bar{\mathcal{H}}}c^{\dagger}_{\mathbf{k}\sigma} \\
&= \langle c_{\mathbf{k}\sigma}(\tau+\beta)c^{\dagger}_{\mathbf{k}\sigma}(0)\rangle \; ,
\end{aligned} \tag{28}$$

we verify that

$$\tilde{g}_{\mathbf{k}\sigma}(\tau<0) = -\tilde{g}_{\mathbf{k}\sigma}(\tau+\beta) \; . \tag{29}$$

The negative sign is a direct consequence of the fermionic algebra. It would be positive if we were dealing with bosons.

We now write $\tilde{g}_{\mathbf{k}\sigma}(\tau)$ as a Fourier series:

$$\tilde{g}_{\mathbf{k}\sigma}(\tau) \equiv \frac{1}{\beta}\sum_{n} \mathrm{e}^{-\mathrm{i}\omega_n\tau}\tilde{G}_{\mathbf{k}\sigma}(\omega_n) \; . \tag{30}$$

In order to satisfy Eq. (29) it is necessary that

$$\mathrm{e}^{-\mathrm{i}\omega_n\beta} = -1 \quad \Rightarrow \quad \beta\omega_n = (2n+1)\pi \; , \quad n = 0, \pm1, \pm2, \ldots \tag{31}$$

The quantities ω_n are called *Matsubara frequencies*. Only odd-integer multiples of π/β appear here for fermions, while the bosonic version involves only even integers.

The "periodicity" relation (29) allows to write the Fourier-series coefficients of Eq. (30), i.e., the frequency-dependent Matsubara GF's, as integrals in the range $[0, \beta]$,

$$\tilde{G}_{\mathbf{k}\sigma}(\omega_n) = \int_0^{\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\tilde{g}_{\mathbf{k}\sigma}(\tau) \; . \tag{32}$$

Thus, only the term with $\tau > 0$ in the τ-ordering contributes, and we can write

$$\tilde{G}_{\mathbf{k}\sigma}(\omega_n) = -\int_0^{\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\langle c_{\mathbf{k}\sigma}(\tau)c^{\dagger}_{\mathbf{k}\sigma}(0)\rangle \; . \tag{33}$$

As before, we formally choose the energy representation to evaluate averages, so that

$$\langle c_{\mathbf{k}\sigma}(\tau)c^{\dagger}_{\mathbf{k}\sigma}(0)\rangle = Z^{-1}\sum_{nm} \mathrm{e}^{-\beta\bar{E}_n}\, \mathrm{e}^{(\bar{E}_n-\bar{E}_m)\tau}\langle n|c_{\mathbf{k}\sigma}|m\rangle\langle m|c^{\dagger}_{\mathbf{k}\sigma}|n\rangle \; . \tag{34}$$

Therefore,

$$\tilde{G}_{\mathbf{k}\sigma}(\omega_n) = -Z^{-1} \sum_{nm} \mathrm{e}^{-\beta \bar{E}_n} \langle n|c_{\mathbf{k}\sigma}|m\rangle \langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle \int_0^\beta \mathrm{d}\tau \, \mathrm{e}^{[\mathrm{i}\omega_n - (\bar{E}_m - \bar{E}_n)]\tau} \; . \tag{35}$$

The integral appearing above is easily solved:

$$\int_0^\beta \mathrm{d}\tau \, \mathrm{e}^{[\mathrm{i}\omega_n - (\bar{E}_m - \bar{E}_n)]\tau} = -\frac{1 + \mathrm{e}^{\beta(\bar{E}_n - \bar{E}_m)}}{\mathrm{i}\omega_n - (\bar{E}_m - \bar{E}_n)} \; . \tag{36}$$

So, we finally obtain

$$\tilde{G}_{\mathbf{k}\sigma}(\omega_n) = Z^{-1} \sum_{nm} \left(\mathrm{e}^{-\beta \bar{E}_n} + \mathrm{e}^{-\beta \bar{E}_m} \right) \frac{\langle n|c_{\mathbf{k}\sigma}|m\rangle \langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle}{\mathrm{i}\omega_n - (\bar{E}_m - \bar{E}_n)} \; . \tag{37}$$

This result is clearly similar to Eq. (14) for retarded and advanced GF's. The only difference is in the denominator, where we have $\mathrm{i}\omega_n$ instead of $\omega \pm \mathrm{i}\eta$. Therefore, with the **same spectral function**, Eq. (17), we can write a generalized GF,

$$G_{\mathbf{k}\sigma}(z) \equiv \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \, \frac{\rho_{\mathbf{k}\sigma}(\varepsilon)}{z - \varepsilon} \; , \tag{38}$$

which is a function of the *complex frequency* z, and may appear in any one of the particular cases

$$G^{\pm}_{\mathbf{k}\sigma}(\omega) = G_{\mathbf{k}\sigma}(\omega \pm \mathrm{i}\eta) \; , \tag{39}$$

$$\tilde{G}_{\mathbf{k}\sigma}(\omega_n) = G_{\mathbf{k}\sigma}(\mathrm{i}\omega_n) \; . \tag{40}$$

This unification enables to evaluate only **one** of the GF types, obtaining the others by analytic continuation in the complex-frequency plane. Note that, unlike real-time GF's, the singularities of a Matsubara GF are **discrete** poles on the **imaginary** axis. Without going into mathematical details, we just mention that it can be rigorously demonstrated that it is possible to perform the **analytic continuation** $\mathrm{i}\omega_n \longleftrightarrow \omega \pm \mathrm{i}\eta$.

In summary, we utilized a formal development, based on the assumption that a set of energy eigenvalues and corresponding eigenvectors exist for a system of interacting electrons, in order to determine generic properties of single-particle Green's functions. A central role is played by the spectral function, which provides information about single-particle excitations. But it can only be extracted after actually evaluating the Green's function (in one of its versions). Doing this through exact solution of the energy-eigenvalue problem is not an option for realistic systems. We will explore alternative schemes in the next texts.