

Green's functions and response to external fields

In our study of elementary excitations in the Fermi-liquid regime of an interacting electron system we worked with two GF's, $G_{\mathbf{k}\sigma}(\omega)$ and $D_{\mathbf{q}}(\omega)$. The first one allows to obtain the quasi-particle energy spectrum, while the second gives the spectrum of particle-hole pairs and plasmons, which are the relevant elementary excitations of the system in question. The use of Green's functions can be expanded, generalizing the basic ideas presented for the ones already discussed. In principle, the energy spectrum of any kind of elementary excitation of a physical system (lattice vibrations, spin waves, etc.) can be obtained from the poles of an appropriately defined GF.

Green's functions are also widely used to study the response of physical systems to external fields, in the context of Linear Response Theory. This theory relates response coefficients (magnetic susceptibility, electrical conductivity, etc.) with Green's functions defined for two conveniently chosen operators, one associated to the physical variable that measures the response and the other to the variable that couples with the external field. In the following, we complement our study of GF's focusing on the evaluation of response functions.

Linear Response Theory

Consider a generic physical system, described by the Hamiltonian \mathcal{H} , to which an external field is applied, generating a perturbation Hamiltonian \mathcal{H}_{ext} (which can be time dependent). So, the total Hamiltonian is

$$\mathcal{H}_{\text{tot}} = \mathcal{H} + \mathcal{H}_{\text{ext}} . \quad (1)$$

As we will deal with quantum statistics, we must employ a density-matrix formalism, in which physical quantities are given by thermodynamic averages of the type

$$\langle A \rangle_t^{\text{tot}} = \text{Tr} \rho_{\text{tot}}(t) A . \quad (2)$$

The *density matrix* ρ_{tot} has its time dependence in the Schrödinger picture given by

$$i \frac{d\rho_{\text{tot}}}{dt} = [\mathcal{H}_{\text{tot}}, \rho_{\text{tot}}] . \quad (3)$$

Separating the perturbation, we have

$$\rho_{\text{tot}} \equiv \rho + \rho_{\text{ext}} , \quad (4)$$

ρ being the density matrix in the absence of external field. For thermodynamic equilibrium at temperature T we have (in the canonical ensemble)

$$\rho = Z^{-1} e^{-\beta \mathcal{H}}; \quad Z = \text{Tr} e^{-\beta \mathcal{H}}; \quad \beta = 1/T . \quad (5)$$

As ρ does not depend on time,

$$i \frac{d\rho_{\text{tot}}}{dt} = i \frac{d\rho_{\text{ext}}}{dt} = [\mathcal{H}_{\text{tot}}, \rho_{\text{tot}}] . \quad (6)$$

The commutator may be split up as follows,

$$\begin{aligned} [\mathcal{H}_{\text{tot}}, \rho_{\text{tot}}] &= [\mathcal{H} + \mathcal{H}_{\text{ext}}, \rho + \rho_{\text{ext}}] \\ &= [\mathcal{H}, \rho] + [\mathcal{H}, \rho_{\text{ext}}] + [\mathcal{H}_{\text{ext}}, \rho] + [\mathcal{H}_{\text{ext}}, \rho_{\text{ext}}] . \end{aligned} \quad (7)$$

The first term of the second line in the above equation is zero, since ρ and \mathcal{H} commute. The last term, which is quadratic in the external field, is **neglected** in **Linear Response Theory**. Therefore, we are left with

$$i \frac{d\rho_{\text{ext}}}{dt} = [\mathcal{H}, \rho_{\text{ext}}] + [\mathcal{H}_{\text{ext}}, \rho] . \quad (8)$$

The above expression is written in the Schrödinger picture. Using the *interaction picture* with respect to the **external perturbation**, \mathcal{H} is seen as the *unperturbed* part, and we have the relationship

$$A(t) = e^{i\mathcal{H}t} A^{(S)} e^{-i\mathcal{H}t} , \quad (9)$$

where the superscript (S) indicates an operator in the Schrödinger picture. Applying this transformation to Eq. (8) we can write an equation of motion for $\rho_{\text{ext}}(t)$ (external part of the density matrix in the interaction picture), which has the final form

$$i \frac{d\rho_{\text{ext}}(t)}{dt} = [\mathcal{H}_{\text{ext}}(t), \rho] . \quad (10)$$

This is a first-order differential equation for $\rho_{\text{ext}}(t)$, subjected to the initial condition

$$\rho_{\text{ext}}(-\infty) = 0 , \quad (11)$$

which reflects the implicit assumption that the perturbation is *adiabatically turned on* starting at $t = -\infty$. Equation (10) can be formally integrated, resulting in

$$\rho_{\text{ext}}(t) = -i \int_{-\infty}^t dt' [\mathcal{H}_{\text{ext}}(t'), \rho] . \quad (12)$$

Let us assume that the system's response is measured by the average value of a physical quantity A (not explicitly time dependent), chosen such as to have zero average in the absence of perturbation. Then,

$$\langle A(t) \rangle_{\text{tot}} = \text{Tr} \rho_{\text{tot}}^{(S)}(t) A = \text{Tr} \rho_{\text{ext}}(t) A(t) , \quad (13)$$

or

$$\langle A(t) \rangle_{\text{tot}} = -i \int_{-\infty}^t dt' \text{Tr} [\mathcal{H}_{\text{ext}}(t'), \rho] A(t) . \quad (14)$$

Using the cyclic property of the trace, we obtain

$$\langle A(t) \rangle_{\text{tot}} = -i \int_{-\infty}^t dt' \langle [A(t), \mathcal{H}_{\text{ext}}(t')] \rangle . \quad (15)$$

We now assume that the Hamiltonian describing the external perturbation has the form

$$\mathcal{H}_{\text{ext}}^{(S)} = -B^{(S)} f(t) , \quad (16)$$

where B is an observable of the system, and the external field is represented by the “force” $f(t)$, which is **not** an operator. This form is actually quite general. We can then write

$$\langle A(t) \rangle_{\text{tot}} = i \int_{-\infty}^t dt' \langle [A(t), B(t')] \rangle f(t') . \quad (17)$$

Relationship with Green’s functions

It is easy to see that Eq. (17) can be written as

$$\langle A(t) \rangle_{\text{tot}} = \int_{-\infty}^{\infty} dt' G_{AB}(t-t') f(t') , \quad (18)$$

if we define a Green’s function involving the operators A and B as given by

$$G_{AB}(t-t') = i\theta(t-t') \langle [A(t), B(t')] \rangle . \quad (19)$$

Note that this is a **retarded** GF, defined in terms of a **commutator**, not an anticommutator. This is so because A and B , being observables, conserve the number of particles (in a fermionic system they are composed by an even number of fermion operators).

Generalized Susceptibility

Typically, the system’s response is related to the external field through what is called a *response function* or *generalized susceptibility*, so that

$$\langle A(t) \rangle_{\text{tot}} = \int_{-\infty}^{\infty} dt' \chi_{AB}(t-t') f(t') . \quad (20)$$

The above integral is a convolution in time. So, it is convenient to take the Fourier transform, which allows to write

$$\langle A(\omega) \rangle_{\text{tot}} = \chi_{AB}(\omega) f(\omega) . \quad (21)$$

From Eqs. (18) and (20) we see that the frequency-dependent response function is nothing but a Green’s function of the observables that measure the response and couple with the field, that is,

$$\chi_{AB}(\omega) = G_{AB}(\omega) . \quad (22)$$

Generalization to non-uniform (i.e., position dependent) external field is straightforward:

$$\langle A(\mathbf{r}, t) \rangle_{\text{tot}} = \int_{-\infty}^{\infty} dt' \int d\mathbf{r}' \chi_{AB}(\mathbf{r} - \mathbf{r}', t - t') f(\mathbf{r}', t'). \quad (23)$$

The double convolution makes it convenient to take Fourier transforms both in space and time, which results in

$$\langle A(\mathbf{k}, \omega) \rangle_{\text{tot}} = \chi_{AB}(\mathbf{k}, \omega) f(\mathbf{k}, \omega). \quad (24)$$

It preserves the relationship between susceptibility and GF, i.e.,

$$\chi_{AB}(\mathbf{k}, \omega) = G_{AB}(\mathbf{k}, \omega), \quad (25)$$

where $G_{AB}(\mathbf{k}, \omega)$ is the Fourier transform of

$$G_{AB}(\mathbf{r} - \mathbf{r}', t - t') = i\theta(t - t') \langle [A(\mathbf{r}, t), B(\mathbf{r}', t')] \rangle. \quad (26)$$

A common example is the **magnetic susceptibility**, which relates magnetization (magnetic response) with applied magnetic field. For most systems whose magnetic moments are localized, these moments can be associated to local (atomic) spins. Then, the local magnetization (apart from multiplicative constants) is given by the average value of a spin operator, $\mathbf{M}_i = \langle \mathbf{S}_i \rangle$. The observable that couples with the external field is also the spin, as the Zeeman term in the Hamiltonian is $\mathcal{H}_Z = -\sum_i \mathbf{H}(\mathbf{R}_i, t) \cdot \mathbf{S}_i$. Therefore, the magnetic-susceptibility tensor has components

$$\chi_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j, t - t') = G_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j, t - t') = i\theta(t - t') \langle [S_i^\alpha(t), S_j^\beta(t')] \rangle, \quad (27)$$

where α and β can be x , y or z in three dimensions. The Fourier-transformed version is $\chi_{\alpha\beta}(\mathbf{k}, \omega) = G_{\alpha\beta}(\mathbf{k}, \omega)$.

This is also applicable to the paramagnetic response of conduction electrons, i.e, leaving aside the diamagnetic contribution from orbital degrees of freedom (Landau diamagnetism). Local electron-spin operators are written in fermion representation as

$$S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}), \quad S_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow}, \quad S_i^- = c_{i\downarrow}^\dagger c_{i\uparrow}, \quad (28)$$

with the corresponding Fourier transforms

$$S_{\mathbf{q}}^z = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} (c_{\mathbf{k}+\mathbf{q}\uparrow}^\dagger c_{\mathbf{k}\uparrow} - c_{\mathbf{k}+\mathbf{q}\downarrow}^\dagger c_{\mathbf{k}\downarrow}), \quad S_{\mathbf{q}}^+ = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}\uparrow}^\dagger c_{\mathbf{k}\downarrow}, \quad S_{\mathbf{q}}^- = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}\downarrow}^\dagger c_{\mathbf{k}\uparrow}. \quad (29)$$

We thus see that $G_{\alpha\beta}(\mathbf{k}, \omega)$ will have essentially the same diagrammatic structure as the density-fluctuation GF, $D_{\mathbf{q}}(\omega)$, studied in Text 15. The only difference is that the single-particle lines converging on the external vertices may refer to different spins.

A detailed analysis of the magnetic susceptibility is beyond the scope of this course, being a natural subject of a course on Magnetism.

Kubo Formula

In certain cases it is convenient to express the response in terms of $\dot{B} \equiv dB/dt$, instead of B . Using

$$G_{AB}(t-t') = i\theta(t-t')\langle[A(t), B(t')]\rangle = i\theta(t-t')\langle[A(0), B(t'-t)]\rangle, \quad (30)$$

we obtain the time derivative

$$\frac{dG_{AB}(t-t')}{dt} = i\delta(t-t')\langle[A, B]\rangle - G_{A\dot{B}}(t-t'). \quad (31)$$

Fourier transforming this last equation, and dividing it by $(-i\omega)$ results in

$$G_{AB}(\omega) = -\frac{\langle[A, B]\rangle}{\omega} + \frac{1}{i\omega}G_{A\dot{B}}(\omega). \quad (32)$$

Therefore, the susceptibility can be written in terms of a GF that involves \dot{B} ,

$$\chi_{AB}(\omega) = -\frac{\langle[A, B]\rangle}{\omega} + \frac{1}{i\omega}G_{A\dot{B}}(\omega). \quad (33)$$

This relationship, known as *Kubo formula*, may appear in different explicit forms depending on the specific problem.

We can also separate the susceptibility in its real and imaginary parts. Given that A and B are observables, i.e., Hermitian, their commutator is *anti-Hermitian*. We can write it in terms of a Hermitian operator C as

$$[A, B] \equiv iC. \quad (34)$$

Therefore, $\langle C \rangle$ is real and $\langle[A, B]\rangle = i\langle C \rangle$ is purely imaginary. From Eq. (33) it then follows that

$$\text{Re } \chi_{AB}(\omega) = \frac{\text{Im } G_{A\dot{B}}(\omega)}{\omega}, \quad (35)$$

$$\text{Im } \chi_{AB}(\omega) = -\frac{1}{\omega} [\text{Re } G_{A\dot{B}}(\omega) + \langle C \rangle]. \quad (36)$$

If the applied field does not vary with time, the response is restricted to the zero-frequency susceptibility $\chi_{AB}(\omega = 0)$, also called *static susceptibility*, and simply denoted as χ_{AB} . Considering that $\chi_{AB}(t)$ is real, $\chi_{AB}(\omega = 0)$ is also real. Thus, Eq. (36) results in the condition

$$\text{Re } G_{A\dot{B}}(\omega = 0) = -\langle C \rangle, \quad (37)$$

and Eq. (35) yields the static susceptibility as

$$\chi_{AB} = \lim_{\omega \rightarrow 0} \frac{\text{Im } G_{A\dot{B}}(\omega)}{\omega}. \quad (38)$$

A typical example in this case is the **electric conductivity** of metals. The interaction of an electron with a uniform electric field \mathbf{E} is described by the Hamiltonian

$$\mathcal{H}_{\text{ext}} = e \sum_i \mathbf{r}_i \cdot \mathbf{E} , \quad (39)$$

where i labels each conduction electron. The response is measured by the electric-current density

$$\mathbf{j} = -\frac{e}{V} \sum_i \dot{\mathbf{r}}_i = -\frac{e}{mV} \sum_i \mathbf{p}_i , \quad (40)$$

where V is the system volume. We then have the following correspondence between generic operators A and B and the relevant operators for this specific problem (without any special notation for \mathbf{r} , \mathbf{p} or \mathbf{j} when representing operators):

$$A \rightarrow \mathbf{j} , \quad B \rightarrow -e \sum_i \mathbf{r}_i , \quad \dot{B} \rightarrow -e \sum_i \dot{\mathbf{r}}_i = V \mathbf{j} . \quad (41)$$

Therefore, we also have the correspondence

$$[A, B] \rightarrow \frac{e^2}{mV} \sum_{ij} [\mathbf{p}_i, \mathbf{r}_j] = -i \frac{ne^2}{m} \mathbf{I} , \quad \chi_{AB} \rightarrow \boldsymbol{\sigma} , \quad (42)$$

where \mathbf{I} is the identity matrix, $n = N/V$ is the electron density, and $\boldsymbol{\sigma}$ is the electric-conductivity tensor.

Defining the current-current Green's function

$$\mathbf{G}_{\mathbf{jj}}(t - t') = i\theta(t - t') \langle [\mathbf{j}(t), \mathbf{j}(t')] \rangle , \quad (43)$$

Eqs. (35-36) and (41-42) imply that

$$\text{Re } \boldsymbol{\sigma}(\omega) = \frac{V}{\omega} \text{Im } \mathbf{G}_{\mathbf{jj}}(\omega) , \quad (44)$$

$$\text{Im } \boldsymbol{\sigma}(\omega) = -\frac{1}{\omega} \left[V \text{Re } \mathbf{G}_{\mathbf{jj}}(\omega) - \frac{ne^2}{m} \right] . \quad (45)$$

These relations determine the real and imaginary parts of the frequency-dependent (also called *optical*) conductivity. From Eq. (38) the *static conductivity* $\boldsymbol{\sigma} \equiv \boldsymbol{\sigma}(\omega = 0)$ is given by

$$\boldsymbol{\sigma} = V \lim_{\omega \rightarrow 0} \frac{\text{Im } \mathbf{G}_{\mathbf{jj}}(\omega)}{\omega} . \quad (46)$$

A Fock-space version of the current-density operator may be obtained from second quantization of the quantum mechanical “current” (multiplied by the electron charge):

$$\mathbf{j}(\mathbf{r}) = \frac{i\hbar e}{2m} \sum_s \left\{ \hat{\psi}_s^\dagger(\mathbf{r}) \nabla \hat{\psi}_s(\mathbf{r}) - \left[\nabla \hat{\psi}_s^\dagger(\mathbf{r}) \right] \hat{\psi}_s(\mathbf{r}) \right\} . \quad (47)$$

Here we use the spin label as s instead of σ to avoid confusion with the conductivity. Besides, we again include \hbar explicitly. The Fourier components of $\mathbf{j}(\mathbf{r})$, written in terms of wavevector-dependent fermion operators, are (in the homogeneous case, i.e., plane-wave basis)

$$\mathbf{j}_{\mathbf{q}} = -\frac{e\hbar}{m} \sum_{\mathbf{k}s} \mathbf{k} c_{\mathbf{k}+\mathbf{q},s}^\dagger c_{\mathbf{k}s}. \quad (48)$$

This form makes it possible to deal with an electric field varying both with time and position, with the replacement $\mathbf{G}_{\mathbf{jj}}(\omega) \rightarrow \mathbf{G}_{\mathbf{jj}}(\mathbf{q}, \omega)$. In the uniform limit ($\mathbf{q} = 0$), we recover a familiar form,

$$\mathbf{j} = -\frac{e\hbar}{m} \sum_{\mathbf{k}s} \mathbf{k} c_{\mathbf{k}s}^\dagger c_{\mathbf{k}s} = -e \sum_{\mathbf{k}s} \mathbf{v}_{\mathbf{k}} \hat{n}_{\mathbf{k}s}, \quad (49)$$

but we should keep in mind that we now have a current **operator**, depending on the occupation-number **operator**.

Similarly to what was observed for the spin susceptibility, we can infer that the diagrammatic structure of $\mathbf{G}_{\mathbf{jj}}(\omega)$ is directly related to that of the density-fluctuation GF, since once more the external vertices involve creation-annihilation pairs.

It is worth remarking that the relationship between electric conductivity and current-current GF is **exact** (within the limits of Linear Response Theory), in contrast to the calculation based on Boltzmann's equation, which involve independent electrons and the semiclassical approximation. Besides the Coulomb interaction between electrons, it is possible to include electron-phonon and/or electron-impurity interactions into the Feynmann diagrams. However, actual evaluation of the current-current GF may become quite complex if one takes all interactions into account.