FIP10601 – Text 14

Simple approximations from the single-particle Green's function

We begin with the most important (formal) result of Text 13 [Eq. (39)], reproduced below.

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

This is an **exact** expression of the Matsubara GF in terms of a self-energy that contains all the interaction effects. This form can be immediately extended to the retarded and advanced GF's by analytic continuation, as already mentioned.

Based on this result, we will present some simple approximations, illustrating how one can self-consistently *renormalize* the Green's function and the electron-electron interaction.

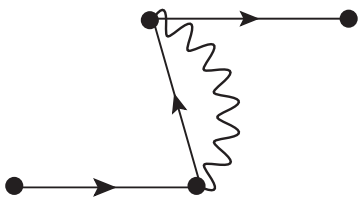
Simplest approximation: 1st-order Σ

Keeping our restriction to the homogeneous limit, the only self-energy diagram that contains a single interaction line is

$\Sigma^{(1)}_{\mathbf{k}\sigma}(\omega_n) =$  . (2)

One can improve on this approximation by considering a *self-consistent* solution in which the GF that appears in the self-energy is *renormalized*, i.e., the original G^0 is replaced by the very G that is being evaluated! Within the diagrammatic technique, this implicitly adds diagrams with self-energy parts inserted in this internal line, but we do not have to explicitly evaluate these additional diagrams. Now the problem becomes self-consistent, as G depends on Σ which in turn depends on G.

Let us make a more detailed analysis of this diagram, which is easier to do with its time version instead of the frequency one. It should be noted that the interaction U is taken as instantaneous. So, the perturbation expansion associates a single time to each $\mathcal{H}_1$ operator, and therefore to the four fermion operators that compose it. Hence, the internal GF has **zero time**. This poses a problem, because the time order is not defined for zero time. It is easier to interpret the diagram if we suppose a retarded Coulomb interaction, so that the "scattering" of each electron occurs at slightly different times. Then we may redraw the diagram (adding the external vertices) as shown below, with the time difference between the internal vertices exaggerated for clarity (time is supposed to grow from left to right).

 (3)

Taking into account that an electron GF for propagation *backwards* in time (annihilation before creation) corresponds to a **hole** propagation forward in time (as observed in Text 12), we can see the latter diagram as the following "sequence of events":

1. an electron is inserted into the system at the initial time (left external vertex);
2. an **electron-hole pair** is spontaneously created, i.e., through a *vacuum fluctuation* (left internal vertex);
3. the inserted electron annihilates the hole (right internal vertex);
4. the spontaneously created electron continues to propagate till the final time (right external vertex).

An **exchange** has thus occurred between the inserted electron and one that leaves the Fermi sea.

This approximation (first-order self-energy with renormalized internal GF) is actually the *Hartree-Fock approximation*. Although we recognize a similarity in the analysis of the exchange term with our evaluation of the Hartree-Fock (HF) ground-state energy (Text 11), the context is slightly different since here we are dealing with single-particle-excitation energies.

From the definition of the Matsubara GF, Eq. (25) of Text 12, we can see that

$$\tilde{g}_{\mathbf{k}\sigma}(0^-) = -\langle \hat{T} c_{\mathbf{k}\sigma}(0^-) c^\dagger_{\mathbf{k}\sigma}(0)\rangle = \langle c^\dagger_{\mathbf{k}\sigma}(0) c_{\mathbf{k}\sigma}(0^-)\rangle = \langle n_{\mathbf{k}\sigma}\rangle \; . \tag{4}$$

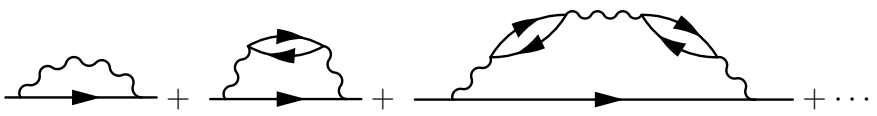
Using this in the expression for the diagram in Eq. (2), it turns out that the HF self-energy is real and independent of frequency. We then have a GF with the same form as the zeroth-order one, but with the energies replaced by

$$\varepsilon^{\rm HF}_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}} - \sum_{\mathbf{k}'} U(\mathbf{k}-\mathbf{k}')\langle n_{\mathbf{k}'\sigma}\rangle \; . \tag{5}$$

These are just independent-electron energies modified by the interaction with the average electron density. Note that the interaction effect involves only electrons in the same spin state. The Hartree term (first-order *tadpole* diagram) would include opposite-spin contributions, but it is null in the homogeneous limit. Equation (4) provides the self-consistency condition, since $\tilde{g}_{\mathbf{k}\sigma}(0^-)$ is given by a sum of all $\tilde{G}_{\mathbf{k}\sigma}(\omega_n)$.

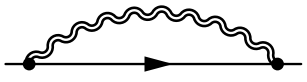
Renormalization of the interaction

Just as we renormalized a G^0 line, we can select an infinite series of diagrams that renormalizes the interaction line. It is easy to see that by adding to the first-order self-energy diagram the second-order one with a *loop* [see Eq. (34) of Text 13] we obtain the first two terms of the series below.

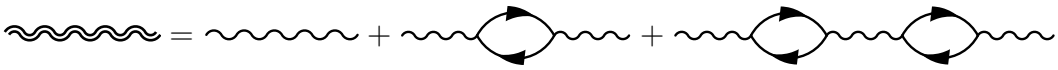


(6)

This series can be replaced by the diagram

 , (7)

where the double line represents a renormalized interaction, given by

 (8)

The simple loop appearing in these diagrams can, in turn, be renormalized, both by renormalization of the G^0 lines and by the inclusion of *connections* between them via interaction lines (*vertex renormalization*). General renormalized loops of this kind are called *polarization parts*. This denomination comes from the fact that these parts can be viewed as the propagation of virtual *electron-hole pairs*, which can also be seen as vacuum polarizations. Equation (8), with zeroth-order polarization parts only, is known as *Random-Phase Approximation* (RPA).

Note that the renormalized interaction line **depends** on frequency. Since an end point of an interaction line is a vertex where a G^0 line ends and another one begins, the interaction line carries a **difference** between two fermionic frequencies, which is a *bosonic* Matsubara frequency. It is customary to use the notation ν_n for bosonic frequencies ($\beta\nu_n = 2n\pi$). A bare interaction line, being instantaneous in time, is **independent** of frequency, meaning that it *carries* **any** frequency. However, explicit frequency dependence appears after insertion of polarization parts, i.e., the interaction ceases to be instantaneous.[1]

The renormalized interaction is usually denoted by $W(\mathbf{q}, \nu_n)$. From Eq. (8), with $\Pi(\mathbf{q}, \nu_n)$ representing the polarization part, we have

$$W(\mathbf{q}, \nu_n) = U(\mathbf{q}) - U(\mathbf{q})\Pi(\mathbf{q}, \nu_n)W(\mathbf{q}, \nu_n) \ , \tag{9}$$

or

$$W(\mathbf{q}, \nu_n) = \frac{U(\mathbf{q})}{1 + U(\mathbf{q})\Pi(\mathbf{q}, \nu_n)} \ , \tag{10}$$

After analytic continuation to real frequencies, we obtain

$$W(\mathbf{q}, \omega) = \frac{U(\mathbf{q})}{1 + U(\mathbf{q})\Pi(\mathbf{q}, \omega)} \equiv \frac{U(\mathbf{q})}{\epsilon(\mathbf{q}, \omega)} \ , \tag{11}$$

Therefore, the renormalized interaction is a **screened** Coulomb potential, and $\epsilon(\mathbf{q}, \omega)$ is the *dielectric constant*.

[1] It is usual to interchange more or less freely references to *imaginary time* (τ) and real time (t), which is justified by the possibility of analytic continuation between Matsubara frequencies and real ones.

The simplest possible calculation of the dielectric constant uses the zeroth-order polarization diagram. We can evaluate this diagram starting with the Matsubara formulation, when we have

$$\Pi^0(\mathbf{q},\nu_n) = -\frac{1}{\beta}\sum_{\mathbf{k}\sigma}\sum_m \tilde{G}^0_{\mathbf{k}\sigma}(\omega_m)\,\tilde{G}^0_{\mathbf{k}+\mathbf{q},\sigma}(\omega_m+\nu_n)\,. \tag{12}$$

Using the explicit form of the zeroth-order GF, and in the end making the analytic continuation $\mathrm{i}\nu_n \to \omega + \mathrm{i}\eta$, we can show **(EXERCISE)** that

$$\Pi^0(\mathbf{q},\omega) = 2\sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k}+\mathbf{q}}) - f(\varepsilon_{\mathbf{k}})}{\omega - (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) + \mathrm{i}\eta}\,. \tag{13}$$

Substituting this for $\Pi(\mathbf{q},\omega)$ in Eq. (11) results in the so-called *Random Phase Approximation*, in which the dielectric constant is given by

$$\epsilon_{\text{RPA}}(\mathbf{q},\omega) = 1 + U(\mathbf{q})\Pi^0(\mathbf{q},\omega)\,. \tag{14}$$

A further simplification, the *Thomas-Fermi Approximation*, takes the static limit (zero frequency) of the renormalized potential, i.e., $W_{\text{TF}}(\mathbf{q}) = U(\mathbf{q})/\epsilon_{\text{RPA}}(\mathbf{q},0)$, additionally evaluating $\Pi^0(\mathbf{q},0)$ in the long-wavelength limit $q \to 0$. A straightforward calculation (**EXERCISE**) at $T = 0$ yields

$$W_{\text{TF}}(\mathbf{q}) = \frac{4\pi\kappa e^2}{V}\frac{1}{q^2 + q^2_{\text{TF}}}\,, \tag{15}$$

where

$$q_{\text{TF}} \equiv \left(\frac{4m\kappa e^2 k_F}{\pi\hbar^2}\right)^{1/2} \tag{16}$$

is known as the *Thomas-Fermi wavevector*. Note that we reinserted $\hbar$ as the relative factor between energy and frequency in order to have the correct physical unit of wavevectors.

From the above result it is again straightforward to obtain the modified Coulomb interaction in position space, which has the form

$$W_{\text{TF}}(\mathbf{r}) = \frac{\kappa e^2}{r}\mathrm{e}^{-q_{\text{TF}}r}\,. \tag{17}$$

Here we recognize a (static) screened Coulomb potential, with screening lenght $1/q_{\text{TF}}$.

Just to have an idea of order of magnitude, we can evaluate q_{TF} assuming an "ideal" Hartree-Fock electron density for a uniform system, which corresponds to $r_s = 4.83$, as obtained in Text 11. We then find a screening lenght of the order of typical interatomic distances in solids, revealing that the Coulomb interaction between single-particle excitations in a metal is both weak and short-ranged in comparison to the bare electron-electron interaction.

In summary, we exemplified how zeroth-order Greens functions or the bare Coulomb interactions are renormalized when we take into account specific series of diagrams for the single-particle Green's function. This was done starting from the simplest (first-order) self-energy diagram. We just mention that the next natural step is to take this diagram and renormalize **both** the G^0 line to G and the U line to W, which is known as **GW approximation**. We will not develop any further details in this context, as it would go beyond our aim here, which is to present the basic aspects related to the study of electronic interactions in solids.