FIP10601 – Text 15

Elementary excitations in the interacting-electron system

Single-particle excitations

Let us go back to the general form of the Matsubara Green's function, Eq. (40) of Text 13, that we rewrite as

$$\tilde{G}_{\mathbf{k}\sigma}(\omega_n) = \frac{1}{\mathrm{i}\omega_n - [\bar{\varepsilon}_{\mathbf{k}} + \Sigma_{\mathbf{k}}(\omega_n)]}\,, \tag{1}$$

where $\bar{\varepsilon}_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$. For simplicity, we eliminate the spin subscript from the self-energy, as we will not consider the possibility of magnetic order.

We now take the analytically continued version (real frequencies), and separate real and imaginary parts of the self-energy as

$$\Sigma_{\mathbf{k}}(\omega) \equiv \Delta_{\mathbf{k}}(\omega) - \mathrm{i}\,\Gamma_{\mathbf{k}}(\omega)\,, \tag{2}$$

where $\Delta_{\mathbf{k}}$ and $\Gamma_{\mathbf{k}}$ are real functions. We then have

$$G_{\mathbf{k}\sigma}(\omega) = \frac{1}{\omega - \bar{\varepsilon}_{\mathbf{k}} - \Delta_{\mathbf{k}}(\omega) + \mathrm{i}\Gamma_{\mathbf{k}}(\omega)}\,. \tag{3}$$

The imaginary part of the denominator is, in principle, finite, eliminating the need to include a term $\mathrm{i}\eta$ that was necessary in the non-interacting case. So, the GF is retarded or advanced according to the sign of $\Gamma_{\mathbf{k}}$ (respectively, positive or negative).

For a given $\mathbf{k}$, the real part of the denominator in Eq. (3) is zero for some real frequency $\omega \equiv \xi_{\mathbf{k}}$ such that

$$\xi_{\mathbf{k}} - \bar{\varepsilon}_{\mathbf{k}} - \Delta_{\mathbf{k}}(\xi_{\mathbf{k}}) = 0\,. \tag{4}$$

Expanding the denominator of Eq. (3) around $\omega = \xi_{\mathbf{k}}$, we can rewrite that equation as

$$G_{\mathbf{k}\sigma}(\omega) = \frac{z_{\mathbf{k}}}{\omega - \xi_{\mathbf{k}} + \mathrm{i}\,\gamma_{\mathbf{k}}} + (\text{non-singular terms})\,, \tag{5}$$

where

$$z_{\mathbf{k}}^{-1} = 1 - \frac{\partial}{\partial\omega}\Delta_{\mathbf{k}}(\omega)\bigg|_{\omega=\xi_{\mathbf{k}}}\,, \tag{6}$$

and we have assumed that the imaginary part of the self-energy is weakly dependent on frequency, replacing it by $\Gamma_{\mathbf{k}} \equiv \Gamma_{\mathbf{k}}(\xi_{\mathbf{k}})$ and defining $\gamma_{\mathbf{k}} \equiv z_{\mathbf{k}}\Gamma_{\mathbf{k}}$.

We see that the GF has poles at frequencies whose real parts are $\xi_{\mathbf{k}}$, so that these are the energies of single-particle excitations with the corresponding wavevectors (and spin σ). To have some insight on the nature of these excitations we must look at their distribution in energy (frequency).

Spectral function

As we saw earlier, the retarded and advanced GF's have spectral representations of the form

$$G^{\pm}_{\mathbf{k}\sigma}(\omega) = \int \mathrm{d}\varepsilon \frac{\rho_{\mathbf{k}\sigma}(\varepsilon)}{\omega - \varepsilon \pm \mathrm{i}\eta} \quad \Rightarrow \quad \rho_{\mathbf{k}\sigma}(\omega) = \mp \frac{1}{\pi} \operatorname{Im} G^{\pm}_{\mathbf{k}\sigma}(\omega) \,. \tag{7}$$

For $G_{\mathbf{k}\sigma}(\omega)$ as given by Eq. (5), the non-singular terms being usually dropped, the spectral function (or spectral density) $\rho_{\mathbf{k}\sigma}(\omega)$ becomes

$$\rho_{\mathbf{k}\sigma}(\omega) = -\mathrm{sgn}(\gamma_{\mathbf{k}}) \, \frac{1}{\pi} \operatorname{Im} G_{\mathbf{k}\sigma}(\omega) \,, \tag{8}$$

which yields

$$\rho_{\mathbf{k}\sigma}(\omega) = z_{\mathbf{k}} \, \frac{1}{\pi} \frac{|\gamma_{\mathbf{k}}|}{(\omega - \xi_{\mathbf{k}})^2 + \gamma_{\mathbf{k}}^2} \,. \tag{9}$$

This spectral density is a Lorentzian distribution with center at $\omega = \xi_{\mathbf{k}}$ and width $|\gamma_{\mathbf{k}}|$, while $z_{\mathbf{k}}$ plays the role of a spectral-weight renormalization factor.

For non-interacting electrons the self-energy goes to zero, and the spectral density becomes a Dirac delta-function centered at the energy $\bar{\varepsilon}_{\mathbf{k}}$, consistent with what was obtained directly from the zeroth-order GF. Therefore, a delta-type spectral function is characteristic of a (non-interacting) **particle**. In this case, as the spectral distribution has zero width in frequency, there is no time dependence, meaning that the particle has infinite lifetime.

Turning on the interaction, the spectral-function peak broadens (and its center shifts to the renormalized energy $\xi_{\mathbf{k}}$). If the spectral function still shows a fairly well defined peak, the excitation is viewed as a (fermionic) ***quasi-particle*** (of wavevector $\mathbf{k}$, spin σ, and energy $\xi_{\mathbf{k}}$), which has a **finite lifetime** $\gamma_{\mathbf{k}}^{-1}$.

Fermi liquid

A fermion system presenting a quasi-particle spectrum which evolves continuously from the non-interacting-particle spectrum as the interaction is adiabatically *turned on* is said to be a *normal Fermi liquid* (or simply Fermi liquid).

Fermi surface

The most striking feature of a Fermi gas (non-interacting particles) is the existence of a **Fermi surface** (at $T = 0$). It is characterized by a **discontinuity** in the average occupation number of electronic states between the inner and outer parts of this constant-energy surface in $\mathbf{k}$-space defined by $\varepsilon_{\mathbf{k}} = \varepsilon_F$.

A question is then in order: **Does the concept of a Fermi surface make sense for a Fermi liquid, that is, for interacting electrons?**

We must bear in mind that $\xi_{\mathbf{k}}$ is an excitation energy which corresponds, in the non-interacting limit, to a single-electron energy relative to the chemical potential, and the latter becomes the Fermi energy at $T = 0$. Then $\xi_{\mathbf{k}} > 0$ must correspond to *electron-like* quasi-particles, while $\xi_{\mathbf{k}} < 0$ must refer to *hole-like* quasi-particles. This is sufficient to show that **the concept of a Fermi surface remains applicable to the interacting system**: it is the surface in **k**-space for which $\xi_{\mathbf{k}} = 0$. Note that, consistently with this definition, the non-interacting Fermi surface may be written as $\bar{\varepsilon}_{\mathbf{k}} = 0$.

Given that the negative-time GF for electrons can be interpreted as a positive-time GF for holes, we associate $\gamma_{\mathbf{k}} > 0$ (retarded GF) to electron-like quasi-particles, and $\gamma_{\mathbf{k}} < 0$ (advanced GF) to hole-like quasi-particles. Therefore, **the imaginary part of the self-energy becomes zero at the FS**. The most interesting implication of this property is that low-energy quasi-particles (close to the FS) tend to have very large lifetimes ($\gamma_{\mathbf{k}} \to 0$).

We can view the connection between single-particle Green's functions and the above-mentioned discontinuity of the average occupation number at the FS by trying to explicitly evaluate this average. It can be done starting from the exact relationship

$$\langle n_{\mathbf{k}\sigma} \rangle = \tilde{g}_{\mathbf{k}\sigma}(\tau = 0^-) \,, \tag{10}$$

already used in our discussion of the HF approximation. From the Fourier-series relation, Eq. (30) of Text 12, we have that

$$\tilde{g}_{\mathbf{k}\sigma}(0^-) \equiv \frac{1}{\beta} \sum_n \mathrm{e}^{\mathrm{i}\omega_n 0^+} \tilde{G}_{\mathbf{k}\sigma}(\omega_n) \,. \tag{11}$$

Now, employing the spectral representation (7) in its Matsubara version gives us

$$\langle n_{\mathbf{k}\sigma} \rangle = \int \mathrm{d}\varepsilon \, \rho_{\mathbf{k}\sigma}(\varepsilon) \frac{1}{\beta} \sum_n \frac{\mathrm{e}^{\mathrm{i}\omega_n 0^+}}{\mathrm{i}\omega_n - \varepsilon} \,. \tag{12}$$

Conveniently choosing a contour C in the complex plane of a variable z (complex frequency), it can be shown that

$$\frac{1}{\beta} \sum_n \frac{\mathrm{e}^{\mathrm{i}\omega_n 0^+}}{\mathrm{i}\omega_n - \varepsilon} = - \oint_C \frac{\mathrm{d}z}{2\pi\mathrm{i}} \, \frac{\mathrm{e}^{z\,0^+} \, f(z)}{z - \varepsilon} = f(\varepsilon), \tag{13}$$

where $f(\varepsilon)$ is the Fermi function, written as $\left(\mathrm{e}^{\beta\varepsilon} + 1\right)^{-1}$, i.e., without explicitly including the chemical potential because the energies are relative to μ. The first equality in Eq. (13) comes from the narrow contour "around" the imaginary axis in the left plot of Fig. 1, and is based on the fact that $f(z)$ has poles on the imaginary axis (with residue $1/\beta$) wherever $z = \mathrm{i}\omega_n$. The second equality corresponds to the split contour of the other plot, for which a single pole exists at the real frequency ε. Note that the relevant part of the integration is along the straight lines parallel to the imaginary axis, since the closing arcs in all contours are at $|z| \to \infty$, where the integrand goes to zero. This is guaranteed by the factor $\mathrm{e}^{z\,0^+}$, where $0+$ must be interpreted as a small positive "time" that is taken to zero in the end.

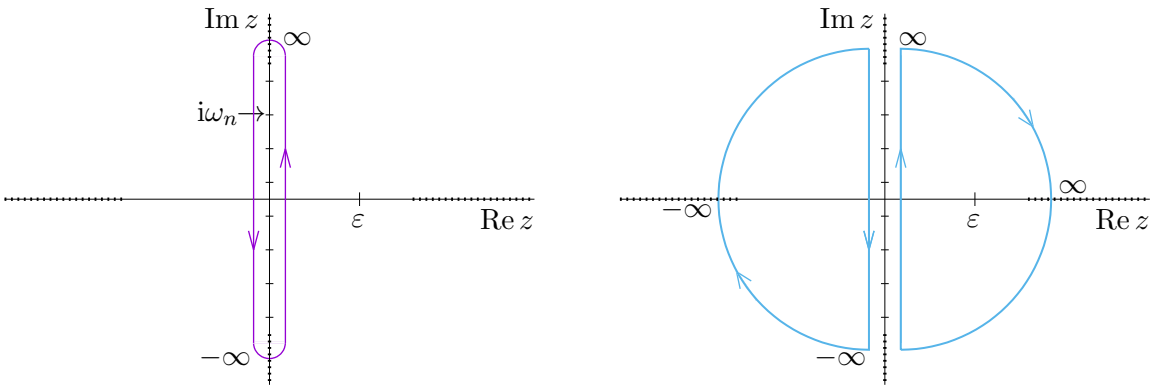

Figure 1: Contour schemes in the complex z plane corresponding to the first and second equalities of Eq. (13) (left and right graphics, respectively). Dots on axis sections far from the origin indicate that these regions are scaled down from infinity.

From Eqs. (12) and (13) we conclude that

$$\langle n_{\mathbf{k}\sigma}\rangle = \int \mathrm{d}\varepsilon\, \rho_{\mathbf{k}\sigma}(\varepsilon) f(\varepsilon)\,. \tag{14}$$

For a non-interacting system $\rho_{\mathbf{k}\sigma}(\varepsilon) = \delta(\varepsilon - \bar{\varepsilon}_{\mathbf{k}})$, and one recovers $\langle n_{\mathbf{k}\sigma}\rangle = f(\bar{\varepsilon}_{\mathbf{k}})$, which jumps from 1 to 0 across the FS in the zero-temperature limit. In the presence of interaction, the finite width of $\rho_{\mathbf{k}\sigma}(\varepsilon)$ transfers spectral weight across the FS. On the other hand, the width $\gamma_{\mathbf{k}}$ goes to zero at the FS, so that $\rho_{\mathbf{k}\sigma}(\varepsilon_F) \to z_{k_F}\delta(\varepsilon_F - \xi_{\mathbf{k}})$. Therefore, the FS is still characterized by a **finite jump** of $\langle n_{\mathbf{k}\sigma}\rangle$, but the "step" has a height $z_{k_F} < 1$. The typical behavior is depicted in Fig. 2.

Taking into account that there is a one-to-one correspondence between $\xi_{\mathbf{k}}$ in the Fermi liquid and $\bar{\varepsilon}_{\mathbf{k}}$ in the Fermi gas, as shown by Eq.(4), **the k-space volume enclosed by the FS is the same as in the non-interacting case** (*Luttinger's Theorem*). This does **not** mean that the FS shape is also preserved, although it should happen in the homogeneous limit (spherical FS).

As a wrapping-up remark, we want to emphasize that what we have learned about the Fermi-liquid state allows us to infer that, despite the presence of electron-electron interactions, the low-energy elementary excitations in a metal behave very much like free electrons! In a sense, this is an *a posteriori* justification for the relative success of the free-electron approximation, provided we reinterpret it as describing quasi-particles of a Fermi liquid.

It is also noteworthy that our study of transport problems through the Boltzmann equation can be applied to Fermi-liquid quasi-particles. In this context, $\gamma_{\mathbf{k}}$ ($\sim \gamma_{k_F}$) can be seen as the inverse of a *relaxation time* $\tau_{\mathrm{e-e}}$ due to the electron-electron interaction. As we have seen for the electron gas, all quantities related to the Fermi surface tend to depart from their ground-state values quadratically on temperature. This qualitative argument can be corroborated by an explicit calculation of $\gamma_{\mathbf{k}}$ taking into account second-order self-energy

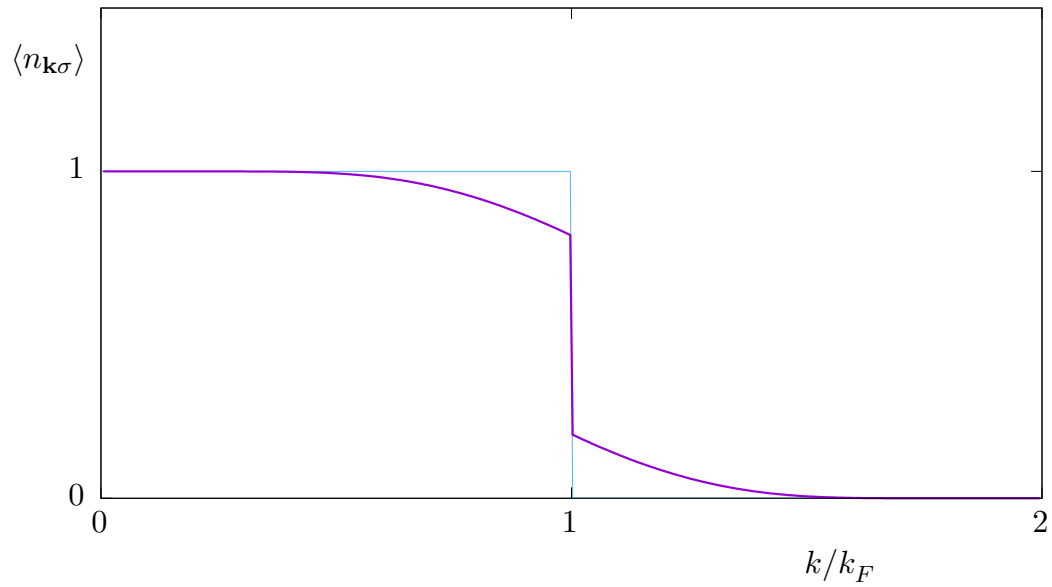

Figure 2: Schematic representation of the average occupation number in a Fermi-liquid. The discontinuity at the Fermi surface has a height $z_{k_F} < 1$.

diagrams (that is, beyond Hartree-Fock). Such a calculation (not shown here) clearly reveals the T^2 behavior for $T \ll T_F$. The resulting variation of $\tau_{\mathrm{e-e}}$ with temperature generates a term proportional to T^2 in the electrical resistivity, which is dominant at low temperatures, when the phonon contribution becomes very small (as we will see latter). This T^2 behavior is observed in resistivity measurements, serving as "signature" of a Fermi-liquid state.

In the above discussion we took for granted the existence of quasi-particle excitations in thermodynamic equilibrium in a Fermi liquid at finite temperature. If we think of *heating up* the system starting from the ground-sate, conservation of the total number of particles implies that we must have the same number of electron-like and hole-like excitations, in the same way as we have equal numbers of electrons and holes in a Fermi gas. The low-energy excitations of the system are still referred to as *electron-hole* excitations, even though we actually have *quasi-electrons* and *quasi-holes*. Next we will see that there are excitations of a different nature at higher energies.

Collective excitations

In addition to particle-hole excitations, which involve independent quasi-particles, a system of interacting electrons also has collective excitations. These two kinds of excitations have a common characteristic: both conserve the number of particles. To describe them, we define a new GF involving the spatial density of electrons.

As we saw in Text 10, the operator associated to the electron density is written in terms of *field operators* (creation and annihilation in coordinate space) as

$$\hat{\rho}(\mathbf{r}) = \sum_{\sigma} \hat{\rho}_{\sigma}(\mathbf{r}) \,, \qquad \hat{\rho}_{\sigma}(\mathbf{r}) = \hat{\psi}^{\dagger}_{\sigma}(\mathbf{r})\hat{\psi}_{\sigma}(\mathbf{r}) \,. \tag{15}$$

To make contact with our formulation in reciprocal space, we can express $\hat{\rho}(\mathbf{r})$ in terms of its Fourier components,

$$\hat{\rho}(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{q}} \mathrm{e}^{\mathrm{i}\mathbf{q}.\mathbf{r}} \hat{\rho}_{\mathbf{q}} \,, \tag{16}$$

where

$$\hat{\rho}_{\mathbf{q}} = \int \mathrm{d}\mathbf{r}\, \mathrm{e}^{-\mathrm{i}\mathbf{q}.\mathbf{r}} \hat{\rho}(\mathbf{r}) \,. \tag{17}$$

In the homogeneous limit, when Bloch functions become plane waves, so that $c_{\mathbf{k}\sigma}$ and $\psi_{\sigma}(\mathbf{r})$ are related by a simple Fourier transform, it follows that

$$\hat{\rho}_{\mathbf{q}} = \sum_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q},\sigma} \,, \tag{18}$$

and its conjugate is

$$\hat{\rho}^{\dagger}_{\mathbf{q}} = \sum_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k}\sigma} \,. \tag{19}$$

Note that

$$\langle \hat{\rho}_{\mathbf{q}} \rangle = \langle \hat{\rho}^{\dagger}_{\mathbf{q}} \rangle = \sum_{\mathbf{k}\sigma} \langle \hat{n}_{\mathbf{k}\sigma} \rangle \delta_{\mathbf{q}\mathbf{0}} \equiv \langle \hat{N} \rangle \delta_{\mathbf{q}\mathbf{0}} \,, \tag{20}$$

where $\langle \hat{N} \rangle$ represents the average total number of electrons, which must be equal to N. From these relationships, we can define a (Matsubara) GF of the form

$$\tilde{D}_{\mathbf{q}}(\tau) = -\left[\langle \hat{T} \hat{\rho}_{\mathbf{q}}(\tau) \hat{\rho}^{\dagger}_{\mathbf{q}}(0) \rangle - \langle \hat{N} \rangle^2 \delta_{\mathbf{q}\mathbf{0}} \right] \,, \tag{21}$$

describing **fluctuations** of the electron density. $\tilde{D}_{\mathbf{q}}$ is a **bosonic** GF since the operator $\hat{\rho}_{\mathbf{q}}$ involves products of two fermion operators.

We can develop a perturbative treatment of $\tilde{D}_{\mathbf{q}}(\tau)$ following the general lines presented in Text 13 for the single-particle GF. The basic difference is that the *external vertices* are now points where a $\tilde{G}^0$ line begins and another one ends, as they represent creation-annihilation pairs. The zeroth-order diagram is thus exactly what we named (zeroth-order) *polarization part* in the first sections of this Text. There is also a disconnected diagram in which each external vertex has a single-particle line closing on itself. But this (after full renormalization of these closed lines) is canceled by the term $\langle \hat{N} \rangle^2$ that appears in the definition of $\tilde{D}_{\mathbf{q}}$. All possible insertions into the zeroth-order diagram lead to a complete polarization part, $\Pi(\mathbf{q}, \nu_n)$. In addition, polarization parts may be connected by interaction lines, generating the series

$$\tilde{D}_{\mathbf{q}}(\nu_n) = \Pi(\mathbf{q},\nu_n) - \Pi(\mathbf{q},\nu_n)U(\mathbf{q})\Pi(\mathbf{q},\nu_n) + \Pi(\mathbf{q},\nu_n)U(\mathbf{q})\Pi(\mathbf{q},\nu_n)U(\mathbf{q})\Pi(\mathbf{q},\nu_n) + \ldots \tag{22}$$

The diagrammatic representation of the r.h.s. of the above equation is very similar to that of Eq. (8) of Text 14, except that it begins and ends with $\Pi(\mathbf{q}, \nu_n)$ instead of $U(\mathbf{q})$. Like in that case, it can be turned into a Dyson's equation, and the result is

$$\tilde{D}_{\mathbf{q}}(\nu_n) = \frac{\Pi(\mathbf{q}, \nu_n)}{1 + U(\mathbf{q})\Pi(\mathbf{q}, \nu_n)} \; . \tag{23}$$

Converting to real frequency (retarded function), we have

$$D_{\mathbf{q}}(\omega) = \frac{\Pi(\mathbf{q}, \omega)}{1 + U(\mathbf{q})\Pi(\mathbf{q}, \omega)} = \frac{\Pi(\mathbf{q}, \omega)}{\epsilon(\mathbf{q}, \omega)} \; , \tag{24}$$

which involves the dielectric constant as defined when we discussed the screening of interactions. From the above relation we see that excitation energies of the interacting-electron system (with conservation of particle number) are given by ***zeros*** of its dielectric constant, which generate poles of $D_{\mathbf{q}}(\omega)$.

In the non-interacting limit, Eq. (24) shows that $D^0_{\mathbf{q}}(\omega) = \Pi^0(\mathbf{q}, \omega)$, whose poles occur at $\omega = \varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}$. What happens to these poles in the interacting system? They are not poles of $D_{\mathbf{q}}(\omega)$, since they cancel out between numerator and denominator in Eq. (24). The actual poles, as we noted before, are given by the zeros of the dielectric function. In the Random Phase Approximation (RPA), introduced in Text 14, one uses the zeroth-order polarization part to evaluate the dieletric function. Then, using the expression previously obtained for Π^0, Eq. (14) of Text 14, we end up with the condition

$$2\,U(\mathbf{q}) \sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k}}) - f(\varepsilon_{\mathbf{k}+\mathbf{q}})}{\omega - (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}})} = 1 \; . \tag{25}$$

Figure 3 shows a schematic plot of the left-hand side of this last equation as a function of frequency, with artificially discretized band energies (dashed lines) for the sake of clarity.

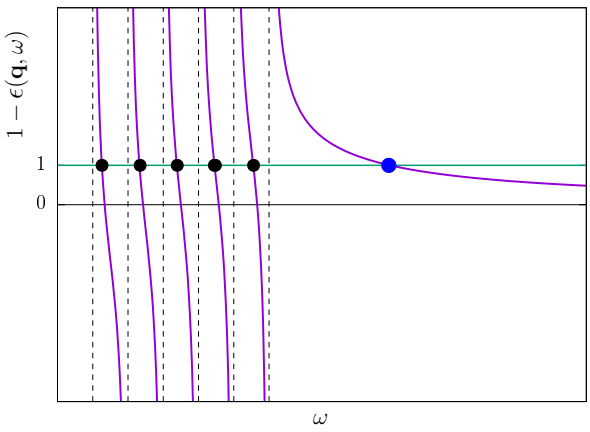

Figure 3: Schematic plot of the left-hand side of Eq. (25) for a small value of $\mathbf{q}$, indicating the points where Eq. (25) is verified. The high-frequency solution, outside the particle-hole region, corresponds to a plasmon excitation.

Note that there is a solution of Eq. (25) between any consecutive poles of $D^0_{\mathbf{q}}(\omega)$ (vertical dashed lines). Therefore, in the macroscopic limit, when these poles have a continuous distribution, the spectrum of particle-hole excitations coincides with the non-interacting one.

However, it is clear from Fig. 3 that there is another solution, for an energy well above the particle-hole continuum. This is a collective mode, whose frequency can be easily evaluated in the long-wavelength limit ($q \to 0$). After some manipulation of the wavevector sum in Eq. (25), we end up with a single Fermi function in the numerator and a difference of squares in the denominator. Then, for small q values, we can neglect the square of the energy difference against ω^2, obtaining **(EXERCISE)**, for a parabolic band with effective mass m^*,

$$\Pi^0(\mathbf{q},\omega) \simeq -\frac{Nq^2}{m^*\omega^2} \; , \tag{26}$$

where N is the total number of electrons. Using the Fourier transform of the Coulomb potential (Text 11), $U(\mathbf{q}) = 4\pi\kappa e^2/Vq^2$, the $q \to 0$ limit of Eq. (25) becomes

$$\frac{4\pi n\kappa e^2}{m^*\omega^2} = 1 \; , \tag{27}$$

where $n = N/V$, the electron density. Therefore, collective excitations of long wavelength occur with a characteristic frequency $\omega = \omega_p$, defined as

$$\omega_p \equiv \left(\frac{4\pi n\kappa e^2}{m^*}\right)^{1/2} \; . \tag{28}$$

It is called *plasma frequency*, and the corresponding oscillation mode is called a *plasmon*.

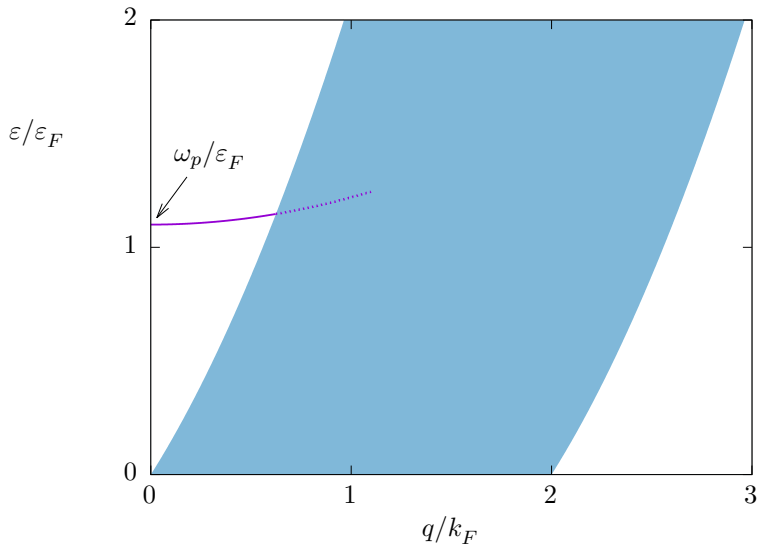

Figure 4: Schematic representation of the Fermi-liquid excitation spectrum, with the continuum of electron-hole excitations (shaded area) and the plasmon line.

Numerical estimation for densities of $10^{22}-10^{23}$ el/cm^3 and m^* near the electron mass yields ω_p with an order of magnitude in the range $10^{15}-10^{16}\,\mathrm{s}^{-1}$, corresponding to energies of the order of 1 to 10 eV. This is the same order of magnitude of the Fermi energy! Plasmons are therefore high-energy excitations.

A more detailed calculation shows that the plasmon energies grow with q^2 from the initial value ω_p. In addition, the imaginary part of the plasmon pole becomes finite when $\omega(q)$ enters the region in which high-energy electron-hole excitations exist, indicating that plasmon modes decay into electron-hole pairs. A schematic representation of both kinds of elementary excitations is shown in Fig. 4. The plasmon line is drawn with dots in the region where plasmons becomes unstable.

Fermi-liquid instabilities

In certain situations, the Fermi-liquid characteristics, i.e., existence of a Fermi surface and low-energy single-particle excitations, are not observed. In such cases, the Fermi-liquid state is **unstable**, and the true ground state (as well as excited states in thermodynamic equilibrium) are of a different nature. The basic point is that the ground-state cannot be viewed as evolving continuously from the non-interacting one.

This can happen, for example, in the presence of additional interactions that significantly change the ground state. In particular, strong *electron-phonon* interaction may cause self-trapping of an electron in lattice deformations induced by the electron itself (localized *polaron*), while weak electron-phonon interaction may generate an *effective* attractive interaction between electrons leading to the establishment of a *superconducting* state at sufficiently low temperatures. We will address the electron-phonon interaction and superconductivity in Texts 16 and 18.

Other cases of Fermi-liquid instability involve narrow-band systems, in which electrons have low mobility. Screening is then not efficient, leaving strong local interactions. The instabilities can be against the establishment of *magnetic order* and/or the occurrence of a *metal-insulator transition*. Here one enters the field of the so-called *strongly correlated electron systems*, where substantially different approaches need to be employed, as will be briefly discussed in the following.

Brief introduction to strongly correlated electron systems

Our perturbative approach to the electron-electron interaction led to the concept of Fermi liquid, which is not substantially different from the Fermi gas. In good part, this was due to the assumed mobility of the electrons. In contrast, if an electron can only hop to a single orbital of a neighboring site, which has a high probability of being occupied by another electron, interaction and spin states become very important.

At the end of Text 10 we have already introduced the Hubbard model, which may be viewed as a prototype model for strongly correlated electrons in solids. Its Hamiltonian is reproduced below.

$$\mathcal{H} = \varepsilon_0 \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} - \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \; . \tag{29}$$

Usually, the hopping t_{ij} is only non-zero between neighboring sites, with a single value t, supposing that all neighbors are equivalent. The Coulomb repulsion is positive ($U > 0$) and the relevant regime corresponds to $U \gg t$. Clearly, the electrons do not move independently. There is correlation due to Pauli's exclusion principle, as hopping can only occur to an empty site or to a site occupied by an electron with **opposite** spin, and also because in the latter case there is an energy cost U.

From the above comments, it is not difficult to infer that at *half filling*, i.e., with one electron per lattice site, the system in the ground state will be an insulator and present antiferromagnetic order. Insulator because any motion will generate a double occupation, which involves an excitation energy U. The antiferromagnetism may be understood as resulting from a second-order perturbative correction in the hopping, i.e., virtual hoppings to a neighboring site and back, which can only happen if the electron that hops and the one occupying the other site have opposite spins.

Another important class of correlated-electron systems are compounds that present two relevant bands: a wide one, usually originated from s and/or p atomic levels, and a narrow one originated from d or f atomic levels. In the usual models, the first one is treated as uncorrelated (i.e., an independent-electron band), while the second is viewed as localized levels, with a strong intra-site Coulomb repulsion. The lack of spherical symmetry in the crystal structure allows for hybridization between the local s an f levels, which is a new important ingredient. With these choices we have the Periodic Anderson Model (PAM), whose Hamiltonian may be written as

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + \varepsilon_f \sum_{i\sigma} n^f_{i\sigma} + U \sum_i n^f_{i\uparrow} n^f_{i\downarrow} + \sum_{\mathbf{k},i} \left(V_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_i} c^\dagger_{\mathbf{k}\sigma} f_{i\sigma} + \mathrm{H.c.} \right) \; , \tag{30}$$

where H.c. stands for *Hermitian conjugate*. The localized f-level, of energy ε_f, is supposed to be placed below the Fermi energy ($\varepsilon_f < \varepsilon_F$), while the doubly occupied state has energy $\varepsilon_f + U > \varepsilon_F$. So, the f levels are singly occupied, and may be viewed as localized spins. We then see that the hybridization will cause the band spins to be locally antiparalell to the f-spin, *screening* this local moment. This is one of the manifestations of the so-called *Kondo effect*, initially addressed in diluted-impurity systems, in which the localized f-electrons belong to diluted impurity atoms inserted into a non-correlated metal. In lattice systems, as modeled by the PAM, we have a competition between the Kondo effect, which tends to screen the local moments, and correlations as those already appearing in the Hubbard model, that may induce magnetic order.

The brief comments presented here just touch a few aspects of the rich field of strongly correlated electron systems, which is a subject of intensive research work.