Electronic Response to External Perturbations

The transport and optical properties of solids are due primarily to the electron system and to a lesser extent to the ions. These properties were discussed in Chapters 24 and 25 without taking the interaction between electrons into account, although its role may be important in some cases. In this chapter we will study the response of the interacting electron system to external perturbations, to an applied electromagnetic field. We will consider first the effect of an external scalar potential and will derive general expressions that relate the dielectric function to the density–density response function and the dynamical structure factor introduced in the previous chapter. This will then allow us to get approximate expressions for the frequency and wave number dependence of the dielectric function. The study of the redistribution of electrons induced by an external charge will lead to a proper description of screening in metals. It will be shown that the optical conductivity can be calculated from the current–current correlation function. Finally, by studying the response of the electron system to an external magnetic field, we will be able to derive an approximate expression for the wave number- and frequency-dependent susceptibility which is the magnetic analog of the dielectric function.

29.1 The Dielectric Function

When a solid is exposed to an external electric field varying in space and time, the relationship between the electric displacement $D$ and the electric field $E$ is not local in space, though it is causal in time. The permittivity must then be expressed in an integral form. The relationship

$$D_\alpha(r, t) = \int dr' \int_{-\infty}^{t} dt' \epsilon_{\alpha\beta}(r - r', t - t') E_\beta(r', t')$$

given in (16.1.50) is valid for isotropic systems. In a crystalline material we have

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\[ D_\alpha(r, t) = \sum_\beta \int dr' \int_{-\infty}^{t} dt' \epsilon_{\alpha\beta}(r, r', t-t') E_\beta(r', t') , \quad (29.1.2) \]

where \( \epsilon_{\alpha\beta}(r, r', t-t') \) depends on \( r \) and \( r' \) separately, not just on their difference. Hence its Fourier transform contains two momentum variables:

\[ \epsilon_{\alpha\beta}(q, q', t-t') = \iint \mathrm{d}r \, \mathrm{d}r' \epsilon_{\alpha\beta}(r, r', t-t') e^{-i q \cdot r} e^{-i q' \cdot r'} . \quad (29.1.3) \]

However, if the position vectors are written as \( r = R_n + u \) and \( r' = R_m + u' \) where \( u \) and \( u' \) are in the primitive cell around the lattice points \( R_n \) and \( R_m \), respectively, the dielectric tensor depends on \( u, u', \) and \( R_n - R_m \) only, owing to the discrete translational invariance of the crystal, and \( q' \) may differ from \(-q\) by a reciprocal-lattice vector \( G \). Taking the Fourier transform with respect to time the relationship

\[ D_\alpha(q, \omega) = \sum_G \sum_\beta \epsilon_{\alpha\beta}(q, -q - G, \omega) E_\beta(q + G, \omega) \quad (29.1.4) \]

is obtained between the Fourier components of the fields. The terms with \( G \neq 0 \) take into account the variations of the fields over atomic distances and yield the so-called local-field corrections. These corrections are usually small and can be neglected, so that the system can be assumed to have full translational symmetry. We then arrive at the usual expression

\[ D_\alpha(q, \omega) = \sum_\beta \epsilon_{\alpha\beta}(q, \omega) E_\beta(q, \omega) . \quad (29.1.5) \]

But, even after this simplification the dielectric function depends on the direction of propagation of the electromagnetic field relative to the crystallographic axes. In what follows we will forget about this and will consider the properties of isotropic materials only.

Decomposing the electric field and the electric displacement into components parallel and perpendicular to the direction of \( q \), their relationship in the general case can be written as

\[ D_\parallel(q, \omega) = \epsilon_\parallel(q, \omega) E_\parallel(q, \omega) , \quad D_\perp(q, \omega) = \epsilon_\perp(q, \omega) E_\perp(q, \omega) , \quad (29.1.6) \]

which means that

\[ D(q, \omega) = \epsilon_\parallel(q, \omega) \frac{q \cdot E(q, \omega)}{q^2} q + \epsilon_\perp(q, \omega) \frac{q \times E(q, \omega)}{q^2} \times q , \quad (29.1.7) \]

i.e., the permittivity tensor has the general form

\[ \epsilon_{\alpha\beta}(q, \omega) = \epsilon_\parallel(q, \omega) \hat{q}_\alpha \hat{q}_\beta + \epsilon_\perp(q, \omega) (\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta) , \quad (29.1.8) \]
where $\hat{q}_\alpha$ is the $\alpha$ component of the unit vector $\hat{q}$ that points in the direction of $q$. The dielectric function is related to the longitudinal component $\epsilon_{||}(q, \omega)$ by

$$\epsilon_r(q, \omega) = \epsilon_{||}(q, \omega)/\epsilon_0. \quad (29.1.9)$$

The dielectric function has been studied previously in Chapter 16 in the framework of the Drude model. The results derived there are, however, valid only in the long-wavelength limit, owing to the approximations inherent to that model. A better approximation will be applied here with the primary aim of studying the role of the electron–electron interaction. This will help us to get a better understanding of how electrons influence each other.

### 29.1.1 Dielectric Response of the Electron System

In order to obtain the dielectric function, we will study what happens in an originally homogeneous electron gas with a neutralizing background when external charges with a spatially inhomogeneous, time-dependent charge density $\rho_{\text{ext}}(r, t)$ are introduced into it. The external charge is related to the electric displacement via Maxwell’s third equation (Gauss’s law):

$$\text{div } D(r, t) = \rho_{\text{ext}}(r, t). \quad (29.1.10)$$

The Coulomb interaction between the external charges and the electrons of the system gives rise to a redistribution of the electrons and induces a charge density $\rho_{\text{ind}}(r, t)$ in the originally homogeneous and neutral system. The electric field $E$ is generated by the total charge density, the sum of external and induced charges,

$$\rho(r, t) = \rho_{\text{ext}}(r, t) + \rho_{\text{ind}}(r, t), \quad (29.1.11)$$

and their relationship is given by

$$\epsilon_0 \text{div } E(r, t) = \rho(r, t). \quad (29.1.12)$$

This field is the negative gradient of the scalar potential $\varphi(r)$,

$$E(r, t) = -\text{grad } \varphi(r, t). \quad (29.1.13)$$

In analogy to this relationship an external potential $\varphi_{\text{ext}}(r)$ can be introduced that is generated by the external charge. It is defined by

$$D(r, t) = -\epsilon_0 \text{grad } \varphi_{\text{ext}}(r, t). \quad (29.1.14)$$

Taking the Fourier transforms of the fields and potentials we find

$$E(q, \omega) = -iq\varphi(q, \omega), \quad D(q, \omega) = -i\epsilon_0q\varphi_{\text{ext}}(q, \omega). \quad (29.1.15)$$

It follows from (29.1.5) that a simple relationship exists between the two potentials:
\[ \varphi(q, \omega) = \frac{\epsilon_0}{\epsilon(q, \omega)} \varphi_{\text{ext}}(q, \omega) = \frac{1}{\epsilon_t(q, \omega)} \varphi_{\text{ext}}(q, \omega). \]  

(29.1.16)

Substitution of (29.1.13) and (29.1.14) into (29.1.12) and (29.1.10), respectively, gives

\[ \epsilon_0 \nabla^2 \varphi(r, t) = -\rho(r, t), \]
\[ \epsilon_0 \nabla^2 \varphi_{\text{ext}}(r, t) = -\rho_{\text{ext}}(r, t). \]  

(29.1.17)

When these relationships are written for the Fourier transforms, they reduce to

\[ \epsilon_0 q^2 \varphi(q, \omega) = \rho(q, \omega), \]
\[ \epsilon_0 q^2 \varphi_{\text{ext}}(q, \omega) = \rho_{\text{ext}}(q, \omega). \]  

(29.1.18)

Comparison of these equations with (29.1.16) yields

\[ \rho(q, \omega) = \frac{1}{\epsilon_t(q, \omega)} \rho_{\text{ext}}(q, \omega) \]  

(29.1.19)

which can be written as

\[ \frac{1}{\epsilon_t(q, \omega)} = \frac{\rho(q, \omega)}{\rho_{\text{ext}}(q, \omega)} = 1 + \frac{\rho_{\text{ind}}(q, \omega)}{\rho_{\text{ext}}(q, \omega)}. \]  

(29.1.20)

If the external charge is expressed in terms of the external potential using (29.1.18), we find

\[ \frac{1}{\epsilon_t(q, \omega)} = 1 + \frac{1}{\epsilon_0 q^2} \varphi_{\text{ext}}(q, \omega). \]  

(29.1.21)

It is often more convenient to use the external, induced, and total number densities, \( n_{\text{ext}}(r), n_{\text{ind}}(r), \) and \( n(r), \) respectively, instead of the corresponding charge densities, where \( \rho_i(r) = -en_i(r). \) Similarly, the quantity \( V_i(r) = -e\varphi_i(r) \) will be used instead of \( \varphi_i \) for both the external and the total potentials. When (29.1.17) is rewritten in terms of these quantities, the Fourier transforms satisfy the relations

\[ V(q, \omega) = \frac{e^2}{\epsilon_0 q^2} n(q, \omega) = \frac{4\pi e^2}{q^2} n(q, \omega), \]
\[ V_{\text{ext}}(q, \omega) = \frac{e^2}{\epsilon_0 q^2} n_{\text{ext}}(q, \omega) = \frac{4\pi e^2}{q^2} n_{\text{ext}}(q, \omega). \]  

(29.1.22)

The dielectric function can then be expressed as

\[ \frac{1}{\epsilon_t(q, \omega)} = 1 + \frac{e^2}{\epsilon_0 q^2} \frac{n_{\text{ind}}(q, \omega)}{V_{\text{ext}}(q, \omega)} = 1 + \frac{4\pi e^2}{q^2} \frac{n_{\text{ind}}(q, \omega)}{V_{\text{ext}}(q, \omega)}. \]  

(29.1.23)

We introduce the quantity \( \Pi(q, \omega) \) defined by
The Dielectric Function

It has a simple physical interpretation. It tells how the electron system responds to the external perturbing potential and how the spatial distribution of electrons is modified in the presence of $V_{\text{ext}}(q,\omega)$. For this reason the quantity $\Pi(q,\omega)$ is called a response function. The inverse of the dielectric function can be written in terms of it as

$$\frac{1}{\epsilon_r(q,\omega)} = 1 + \frac{4\pi e^2}{q^2} \Pi(q,\omega).$$

Thus, the calculation of the dielectric function reduces to calculating this response function.

### 29.1.2 Density–Density Response Function

The function $\Pi(q,\omega)$ was defined by (29.1.24) as the proportionality factor between the charge induced in an interacting electron system and the external perturbing potential. The Hamiltonian of this perturbation can be written in analogy to (28.1.8) in the form

$$\mathcal{H}_1(t) = \sum_i V_{\text{ext}}(r_i, t) = \int V_{\text{ext}}(r, t)n(r) \, dr.$$  

Hence the potential couples to the electron density. In terms of the Fourier transforms we have

$$\mathcal{H}_1(t) = \frac{1}{V} \sum_q V_{\text{ext}}(q, t)n(-q).$$

If the external perturbation is weak and the induced density $n_{\text{ind}}(q,\omega)$ is proportional to the external perturbation, $\Pi(q,\omega)$ can be calculated using linear response theory as a generalized susceptibility. Since the external potential couples to the density and the system responds by modifying its density, the quantity to be considered, $\Pi(q,\omega)$, is the Fourier transform of the density–density response function, also known as the retarded density–density correlation function,

$$\Pi(q,\omega) = -\frac{i}{\hbar} \int_0^\infty d(t-t') e^{i\omega(t-t')-\delta(t-t')} \frac{1}{V} \left\langle \left[ n(q, t), n(-q, t') \right]_- \right\rangle,$$

that is

$$\Pi(q,\omega) = -\frac{i}{\hbar} \int_0^\infty d(t-t') e^{i\omega(t-t')-\delta(t-t')} \frac{1}{V} \left\langle \left[ n(q, t), n(-q, t') \right]_- \right\rangle,$$  

where $\delta$ is a positive infinitesimal. As discussed in Appendix J [see (J.1.53), (J.1.54), (J.1.55), and (J.1.56)] it ensures the adiabatic switching on of the perturbation and hence the correct analytic properties.
The thermal average can be calculated in terms of the matrix elements between the complete set of many-body eigenstates $|\Psi_n\rangle$ of the Hamiltonian that includes the interaction between electrons but not the external perturbation. Using the completeness relation we obtain the spectral representation of the response function:

$$\Pi(r, r', t - t') = -\frac{i}{\hbar} \theta(t - t') \sum_{mn} \frac{e^{-\beta E_n}}{Z} \left[ \langle \Psi_n | n(r, t) | \Psi_m \rangle \langle \Psi_m | n(r', t') | \Psi_n \rangle - \langle \Psi_n | n(r', t') | \Psi_m \rangle \langle \Psi_m | n(r, t) | \Psi_n \rangle \right].$$

(29.1.30)

The time dependence of the operators can be explicitly given in terms of the eigenvalues $E_n$. Interchanging the labels $n$ and $m$ in the second term, the Fourier transform of the response function is

$$\Pi(q, \omega) = \frac{1}{V} \sum_{mn} \left( e^{-\beta E_n} - e^{-\beta E_m} \right) \frac{\langle \Psi_n | n(q) | \Psi_m \rangle \langle \Psi_m | n(-q) | \Psi_n \rangle}{\hbar \omega - E_m + E_n + i\delta}.$$  

(29.1.31)

It will prove convenient to consider the spin-resolved response functions, i.e., the response of electrons with spin $\sigma$ to a perturbation that couples to electrons with spin $\sigma'$. For this we define the response function

$$\Pi_{\sigma\sigma'}(r, r', t - t') = -\frac{i}{\hbar} \theta(t - t') \left[ n_{\sigma}(r, t), n_{\sigma'}(r', t') \right]_-,$$

(29.1.32)

and its Fourier transform with respect to the spatial variable,

$$\Pi_{\sigma\sigma'}(q, t - t') = -\frac{i}{\hbar} \theta(t - t') \frac{1}{V} \left[ n_{\sigma}(q, t), n_{\sigma'}(-q, t') \right]_-,$$

(29.1.33)

where the second-quantized form of the Fourier transform of the density of electrons with spin $\sigma$ is

$$n_{\sigma}(q, t) = \sum_k \tilde{c}_{k\sigma}(t) c_{k + q\sigma}(t).$$

(29.1.34)

Thus $\Pi_{\sigma\sigma'}(q, t - t')$ describes the propagation of an electron–hole pair with momentum $q$ and spin $\sigma'$ that is created at time $t'$. It gives the probability of finding this pair at a later time $t$ with the same momentum and spin $\sigma$. This propagation can be represented pictorially by the diagram shown in Fig. 29.1.

In the simplest case, when the electron–hole pair does not interact with the other electrons of the Fermi sea during its propagation, we get the response function $\Pi_0$ of free electrons. In reality, the electron and the hole can take part in a variety of scattering processes due to electron–electron interaction. This is represented in the diagram by the shaded circle. Although strictly speaking the Feynman diagram technique can be used only for the causal Green
functions, diagrams can help to visualize the contributions to the retarded response function as well. Figure 29.2 shows a few low-order processes in the propagation of electron–hole pairs. The wavy lines represent the interaction.

\[ S(q, \omega) = -\frac{2\hbar}{1 - e^{-\beta \hbar \omega}} \frac{V}{N_e} \text{Im} \Pi(q, \omega), \quad (29.1.35) \]

or, if \( \Pi(q, \omega) \) is expressed through the dielectric function via (29.1.25),

\[ S(q, \omega) = -\frac{2\hbar}{1 - e^{-\beta \hbar \omega}} \frac{V}{N_e} \frac{q^2}{4\pi e^2} \text{Im} \frac{1}{\epsilon_r(q, \omega)}. \quad (29.1.36) \]
The retarded response function $\Pi$ being analytic in the upper half of the complex $\omega$ plane, the real and imaginary parts satisfy the Kramers–Kronig relation

$$\text{Re} \Pi(q, \omega) = \frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \text{Im} \Pi(q, \omega') \frac{\omega' - \omega}{\omega' - \omega} \ d\omega'$$

(29.1.37)

$$= \frac{1}{\pi} \frac{N_e}{2\pi \hbar} \int_{-\infty}^{\infty} \frac{S(q, \omega')}{\omega - \omega'} (1 - e^{-\beta\hbar\omega'}) \ d\omega'.$$

Taking both the real and imaginary parts, the full response function can be written in the form

$$\Pi(q, \omega) = \frac{1}{2\pi \hbar} \frac{N_e}{V} \int_{-\infty}^{\infty} \frac{S(q, \omega')}{\omega - \omega' + i\delta} (1 - e^{-\beta\hbar\omega'}) \ d\omega'.$$

(29.1.38)

Substituting (28.4.92) into this expression we recover the spectral representation of the response function given in (29.1.31).

Since $S(q, \omega)$ satisfies (28.4.104), the response function can be written as

$$\Pi(q, \omega) = \frac{1}{2\pi \hbar} \frac{N_e}{V} \int_{0}^{\infty} S(q, \omega') (1 - e^{-\beta\hbar\omega'}) \left[ \frac{1}{\omega - \omega' + i\delta} - \frac{1}{\omega + \omega' + i\delta} \right] d\omega'.$$

(29.1.39)

Inserting this into (29.1.25) we get

$$\frac{1}{\epsilon(q, \omega)} = 1 + \frac{4\pi e^2}{q^2} \frac{1}{2\pi \hbar} \frac{N_e}{V} \int_{0}^{\infty} S(q, \omega')(1 - e^{-\beta\hbar\omega'})$$

$$\times \left[ \frac{1}{\omega - \omega' + i\delta} - \frac{1}{\omega + \omega' + i\delta} \right] d\omega'.$$

(29.1.40)

At $T = 0$, where the dynamical structure factor is given by (28.4.91), we find

$$\frac{1}{\epsilon(q, \omega)} = 1 + \frac{4\pi e^2}{q^2} \frac{1}{V} \sum_{m} |\langle \Psi_0 | n(q) | \Psi_m \rangle|^2$$

$$\times \left[ \frac{1}{\hbar\omega - E_m + E_0 + i\delta} - \frac{1}{\hbar\omega + E_m - E_0 + i\delta} \right]$$

(29.1.41)

$$= 1 + \frac{4\pi e^2}{q^2} \frac{1}{V} \sum_{m} |\langle \Psi_0 | n(q) | \Psi_m \rangle|^2 \frac{2(E_m - E_0)}{(\hbar\omega + i\delta)^2 - (E_m - E_0)^2}.$$
be taken into account in their full complexity. This requires to solve a complicated many-body problem. The difficulties can partially be circumvented by applying a self-consistent approach.

The full potential felt by the electrons is not the external potential $\varphi_{\text{ext}}$ weakened by the dielectric function. Similarly, for the quantity $V = -e\varphi$ we have $V = V_{\text{ext}}/\epsilon_r$. The internal electric field is the negative gradient of this potential. Since $\epsilon_r$ is related to the internal dynamics of the electron system, the weakening of the external potential inside the system can be interpreted as arising from the screening effect of the dynamically rearranged charges. For this reason $\varphi$ and $V$ are called screened potentials.

When $V_{\text{ext}}$ is replaced in (29.1.23) with $V\epsilon_r$, we have

$$\frac{1}{\epsilon_r(q, \omega)} = 1 + \frac{4\pi e^2}{q^2} \frac{1}{\epsilon_r(q, \omega)} \frac{n_{\text{ind}}(q, \omega)}{V(q, \omega)}, \quad (29.1.42)$$

from which after simple manipulations we obtain

$$\epsilon_r(q, \omega) = 1 - \frac{4\pi e^2}{q^2} \frac{n_{\text{ind}}(q, \omega)}{V(q, \omega)}. \quad (29.1.43)$$

If the function $\Pi(q, \omega)$ is defined by

$$n_{\text{ind}}(q, \omega) = \Pi(q, \omega)V(q, \omega) \quad (29.1.44)$$

as the response to the screened potential, the dielectric function is

$$\epsilon_r(q, \omega) = 1 - \frac{4\pi e^2}{q^2} \tilde{\Pi}(q, \omega). \quad (29.1.45)$$

Comparison with (29.1.25) gives the following relationship between $\Pi(q, \omega)$ and $\Pi(q, \omega)$:

$$\Pi(q, \omega) = \frac{\Pi(q, \omega)}{1 - (4\pi e^2/q^2)\Pi(q, \omega)} = \frac{\Pi(q, \omega)}{\epsilon_r(q, \omega)}, \quad (29.1.46)$$

and the inverse dielectric function can be written as

$$\frac{1}{\epsilon_r(q, \omega)} = 1 + U_{\text{eff}}(q, \omega)\tilde{\Pi}(q, \omega) \quad (29.1.47)$$

with

$$U_{\text{eff}}(q, \omega) = \frac{(4\pi e^2/q^2)}{1 - (4\pi e^2/q^2)\Pi(q, \omega)} = \frac{1}{\epsilon_r(q, \omega)} \frac{4\pi e^2}{q^2}. \quad (29.1.48)$$

Comparison of (29.1.25) with (29.1.47) shows that the dielectric properties of the interacting electron system can be described in two ways. Either the bare Coulomb coupling $4\pi e^2/q^2$ and the full response function $\Pi$ is used, or
the Coulomb interaction is assumed to be screened and then only the response \( \Pi \) to the screened potential has to be considered. This latter approach is more convenient because the screened interaction is short ranged and does not contain the singularities characteristic of the Coulomb potential.

The self-consistent approach can be visualized by the diagrams used to represent the propagation of electron–hole pairs. Let us remark that some of the diagrams seen in Fig. 29.2 can be separated into two disjoint parts by removing a single interaction line. The initial point corresponding to the operator \( n(q,t) \) and the final point corresponding to \( n(-q,t') \) appear in the two distinct pieces. These are called reducible or improper diagrams. A diagram which cannot be broken into unconnected parts by cutting a single interaction line is called irreducible or proper. Such processes are shown in Fig. 29.3.

The reducible diagrams (some low-order ones can be seen in Fig. 29.2) can clearly be constructed by connecting irreducible diagrams by interaction lines in a sequence. If the sum of the contribution of all irreducible diagrams is denoted by \( \Pi(q,\omega) \), then the full response function is the sum of a geometric progression:

\[
\Pi(q,\omega) = \Pi(q,\omega) + \Pi(q,\omega) \frac{4\pi\varepsilon^2}{q^2} \Pi(q,\omega)
\]

\[
+ \Pi(q,\omega) \frac{4\pi\varepsilon^2}{q^2} \Pi(q,\omega) \frac{4\pi\varepsilon^2}{q^2} \Pi(q,\omega) + \cdots
\]

\[
= \frac{\Pi(q,\omega)}{1 - (4\pi\varepsilon^2/q^2)\Pi(q,\omega)}.
\]

Comparing this expression with (29.1.46) we see that \( \Pi \) appearing in the self-consistent approach is in fact the contribution of the irreducible diagrams. \(^1\)

A self-consistent potential can also be introduced for Bloch electrons interacting with a general potential \( U(q) \). The internal dynamics of the system gives rise to screening and the effective interaction between the particles is

\[
U_{\text{eff}}(q,\omega) = \frac{U(q)}{1 - U(q)\Pi(q,\omega)}.
\]

\(^1\) For this reason \( \Pi \) is sometimes called irreducible polarization function or irreducible polarization insertion.
The relation between the full response function and the irreducible one is then

\[
\Pi(q, \omega) = \frac{\tilde{\Pi}(q, \omega)}{1 - U(q)\tilde{\Pi}(q, \omega)}.
\]  

(29.1.51)

### 29.2 Dielectric Function of the Uniform Electron Gas

Having written down general expressions for the dielectric function and the response function \( \Pi(q, \omega) \) of an interacting electron system, we will now attempt to compute its explicit form, its \( q \) and \( \omega \) dependence. The full panoply of many-body theory would be needed if the electron–electron interaction is to be taken into account in its complexity. A reasonable approximate form can be obtained much simpler in the self-consistent treatment when the irreducible part of the response function, \( \tilde{\Pi}(q, \omega) \), is approximated by \( \Pi_0(q, \omega) \), the response function of noninteracting electrons. This latter quantity can be evaluated exactly and can be written in a closed form. Before presenting this result it is useful to get acquainted with a simple semiclassical approach. Finally corrections beyond the self-consistent approach will be considered.

#### 29.2.1 Thomas–Fermi Approximation

When the electron system is exposed to a static (time-independent), spatially slowly varying external potential, both the induced charge and the full (screened) potential \( V(r) \) are also slowly varying in space. We may assume in the spirit of the semiclassical approximation that a local, spatially varying energy \( \tilde{\epsilon}_k(r) \) can be defined, which is the bare energy of an electron shifted by the potential at the position \( r \) of the electron:

\[
\tilde{\epsilon}_k(r) = \epsilon_k + V(r).
\]  

(29.2.1)

This is shown schematically in Fig. 29.4.

---

**Fig. 29.4.** Local displacement of the electron energy in the presence of a spatially slowly varying potential.
Since the chemical potential is constant in space in thermal equilibrium, the Fermi momentum has to vary in space together with the spatial variation of the potential \( V(r) \) in accordance with the relation

\[
\mu = \frac{\hbar^2 k_F^2(r)}{2m_e} + V(r) .
\]  

(29.2.2)

It then follows that

\[
k_F(r) = \frac{\sqrt{2m_e}}{\hbar} [\mu - V(r)]^{1/2} = k_F \left[ 1 - \frac{V(r)}{\mu} \right]^{1/2} .
\]  

(29.2.3)

The electron density has to exhibit a similar spatial variation since according to (16.2.25) there is a unique relationship between the electron density and the Fermi momentum:

\[
n_e(r) = \frac{k_F^3}{3\pi^2} = \frac{k_F^3}{3\pi^2} \left[ 1 - \frac{V(r)}{\mu} \right]^{3/2} .
\]  

(29.2.4)

For weak external potentials a first-order expansion,

\[
n_e(r) = \frac{k_F^3}{3\pi^2} \left[ 1 - \frac{3}{2} \frac{V(r)}{\mu} \right] = \frac{k_F^3}{3\pi^2} - \frac{m_e k_F}{\pi^2 \hbar^2} V(r) ,
\]  

(29.2.5)

gives satisfactory results. One can recognize in the coefficient of \( V(r) \) the electronic density of states at the Fermi energy, and so the induced electron density is given by

\[
n_{\text{ind}}(r) = -\rho(\varepsilon_F) V(r) .
\]  

(29.2.6)

This result has a simple interpretation. When the external potential shifts locally and rigidly, by the same amount, all electron energies, the number of states that are pushed above the chemical potential and become empty is exactly equal to the number of states in a range of width \( V(r) \) around the Fermi energy.

The foregoing calculation was done at temperature \( T = 0 \). The same result is valid at finite temperatures, too. To show this we make use of the fact that at finite temperature the occupation of electron states is given by the Fermi distribution function \( f_0(\tilde{\varepsilon}_k(r)) \), and the local electron density is

\[
n_e(r) = \frac{1}{V} \sum_{k\sigma} f_0(\tilde{\varepsilon}_k(r)) .
\]  

(29.2.7)

The change in the electron density due to the external perturbation, i.e., the induced electron density, is given by the difference

\[
n_{\text{ind}}(r) = \frac{1}{V} \sum_{k\sigma} f_0(\tilde{\varepsilon}_k(r)) - \frac{1}{V} \sum_{k\sigma} f_0(\varepsilon_k)
\]  

\[= \frac{1}{(2\pi)^3} \sum_{\sigma} \int d\mathbf{k} [f_0(\tilde{\varepsilon}_k(r)) - f_0(\varepsilon_k)].
\]  

(29.2.8)
If the external potential is weak compared to the Fermi energy, the function
\( f_0(\varepsilon_k(r)) = f_0(\varepsilon_k + V(r)) \) can be expanded in powers of \( V(r) \). To linear order in the potential we find

\[
\mathcal{n}_{\text{ind}}(r) = \frac{1}{(2\pi)^3} \sum \int d\mathbf{k} \frac{\partial f_0(\varepsilon_k)}{\partial \varepsilon_k} V(r). \tag{29.2.9}
\]

If the integral over \( k \) is converted to an integral over energy and the temperature-dependent corrections in the Sommerfeld expansion [see (16.2.77)] are neglected, the leading term in the expansion gives precisely (29.2.6).

When the Fourier transforms are used,

\[
\mathcal{n}_{\text{ind}}(q) = -\rho(\varepsilon_F)V(q). \tag{29.2.10}
\]

Thus in this approximation, known as the Thomas–Fermi approximation,\(^2\) a \( q \)-independent response function is obtained:

\[
\widetilde{\Pi}(q,\omega) = -\rho(\varepsilon_F), \tag{29.2.11}
\]

which means that the electrons respond locally to the slowly varying external perturbation. By substituting this into (29.1.45) the dielectric function reduces to

\[
\epsilon_r(q) = 1 + \frac{4\pi\varepsilon^2}{q^2} \rho(\varepsilon_F) = 1 + \frac{q_{\text{TF}}^2}{q^2}, \tag{29.2.12}
\]

where the Thomas–Fermi wave number \( q_{\text{TF}} \) has been introduced with the definition

\[
q_{\text{TF}}^2 = \frac{4\pi\varepsilon^2}{\rho(\varepsilon_F)}. \tag{29.2.13}
\]

Its physical meaning will become clear later on.

This result for the long-wavelength limit of the dielectric function is a good approximation for metals. The singularity at \( q = 0 \) is simply the consequence of the fact that a homogeneous electric field cannot be maintained in metals in thermal equilibrium.

### 29.2.2 The RPA

The Thomas–Fermi approach that relies on the semiclassical approximation is valid only for long-wavelength perturbations. It is in this limit that \( \widetilde{\Pi} \) is equal to the negative of the density of states at the Fermi energy. For shorter wavelengths a better approximation is needed. When working with the screened potential and the response to it, one might argue that screening takes into account at least in part the interaction between electrons; moreover, the screened interaction is much weaker than the bare Coulomb interaction and short ranged.\(^3\) Therefore, replacing \( \widetilde{\Pi} \) by its zeroth-order expression, \( \Pi_0 \),

\(^2\) L. H. Thomas, 1927 and E. Fermi, 1928.

\(^3\) As we will see, the \( 1/q^2 \) singularity of the Fourier transform of the Coulomb interaction vanishes when the screened interaction is considered.
might be justified. In this approximation, which for historical reasons is called the RPA,\(^4\) we have
\[
\Pi(q, \omega) = \frac{\Pi_0(q, \omega)}{1 - (4\pi\tilde{e}^2/q^2)\Pi_0(q, \omega)},
\]
(29.2.14)
i.e., the full response is a geometric series whose first term, \(\Pi_0\), corresponds to the free propagation of an electron–hole pair, without scattering processes. The diagram corresponding to \(\Pi_0\) is a simple bubble, also known as the polarization bubble. The higher order terms correspond to a special subset of all possible scattering processes. The electron–hole pair is annihilated in an interaction process creating another electron–hole pair. In the diagrammatic representation, the RPA corresponds to a series of bubbles shown in Fig. 29.5.

\[\text{Fig. 29.5. Graphical representation of the propagation of an interacting electron–hole pair in the RPA}\]

The effective interaction obtained in this approximation,
\[
U_{\text{eff}}(q, \omega) = \frac{U(q)}{1 - U(q)\Pi_0(q, \omega)},
\]
(29.2.15)
can be represented by the diagrams depicted in Fig. 29.6. An infinite series of bubbles appears in the intermediate states. Thus, in the RPA, the effective interaction is mediated by subsequent electron–hole pairs.

\[\text{Fig. 29.6. Processes contributing to the screening of the interaction } U \text{ in the RPA}\]

When this approximation is applied to the dielectric function, it follows from (29.1.44) and (29.1.45) that in the RPA
\[
n_{\text{ind}}(q, \omega) = \Pi_0(q, \omega)V(q, \omega)
\]
(29.2.16)
and
\[
\epsilon_{\tau}^{\text{RPA}}(q, \omega) = 1 - \frac{4\pi\tilde{e}^2}{q^2}\Pi_0(q, \omega).
\]
(29.2.17)

\(^4\) Acronym for random phase approximation.
29.2 Dielectric Function of the Uniform Electron Gas

29.2.3 The Lindhard Dielectric Function

We will now show that $\Pi_0$ can be calculated exactly in closed form and a simple expression can be obtained for the dielectric function in the RPA. The formulas will be derived in two ways: first using elementary considerations of quantum mechanics and then applying the formalism of many-body theory. At a later stage, the results will be generalized to Bloch electrons moving through the periodic potential of the lattice.

Since the Fourier components belonging to different $q$ and $\omega$ values are not mixed in the dielectric response, it is sufficient to consider the change in the electron density caused by a potential

$$V(r,t) = \frac{1}{V} \left[ V(q) e^{i(q \cdot r - \omega t)} e^{\delta t} + V^*(q) e^{-i(q \cdot r - \omega t)} e^{\delta t} \right] \tag{29.2.18}$$

that varies periodically both in space and in time. The infinitesimally small positive $\delta$ ensures the adiabatic switching on of the perturbation.

We will consider a plane-wave state $\psi_k^{(0)}(r) = e^{i k \cdot r / \sqrt{V}}$ of the unperturbed system and study its time evolution due to the disturbance. The perturbed wavefunction $\psi_k(r,t)$ can be expanded in terms of a complete set of states. It is convenient to choose the eigenfunctions of the unperturbed Hamiltonian as this basis set, which in our case means an expansion in terms of plane waves:

$$\psi_k(r,t) = \sum_{k'} \alpha_{k'}(t) \psi_{k'}^{(0)}(r) e^{-i \varepsilon_{k'} t / \hbar} \tag{29.2.19}$$

In the leading, linear order, the perturbing potential mixes the state $\psi_k^{(0)}$ only with the states $\psi_{k+q}^{(0)}$ and $\psi_{k-q}^{(0)}$. The perturbed wavefunction can therefore be looked for in the form

$$\psi_k(r,t) = \psi_k^{(0)}(r) e^{-i \varepsilon_k t / \hbar} + \alpha_{k+q}(t) \psi_{k+q}^{(0)}(r) e^{-i \varepsilon_{k+q} t / \hbar} + \alpha_{k-q}(t) \psi_{k-q}^{(0)}(r) e^{-i \varepsilon_{k-q} t / \hbar} \tag{29.2.20}$$

The coefficient of the first term was chosen to be unity, since the coefficients $\alpha_{k'}(t)$ will be evaluated in lowest order of perturbation theory.

Using (G.2.7) we find

$$\alpha_{k+q}(t) = -\frac{i}{\hbar} \int_{-\infty}^{t} \langle \psi_{k+q}^{(0)} | H_1(t_1) | \psi_k^{(0)} \rangle e^{i (\varepsilon_{k+q} - \varepsilon_k) t_1 / \hbar} dt_1 \tag{29.2.21}$$

where the perturbing Hamiltonian $H_1(t)$ has the same form as (29.1.26), except that here the screened potential $V$ has to be used instead of $V_{\text{ext}}$.

If the space and time dependence of the perturbing potential is given by (29.2.18), the integration over the time variable $t_1$ can be performed. We get
The perturbed wavefunction can thus be written as
\[
\psi_k(r, t) = \psi_k^{(0)}(r)e^{-i\varepsilon_k t/\hbar} \left[ 1 + \frac{1}{V} \frac{V(q)e^{i(q \cdot r - \omega t)}e^{\delta t}}{\hbar \omega - \varepsilon_{k+q} + \varepsilon_k + i\delta} + \frac{1}{V} \frac{V^*(q)e^{-i(q \cdot r - \omega t)}e^{\delta t}}{-\hbar \omega - \varepsilon_{k-q} + \varepsilon_k + i\delta} \right].
\]  
(29.2.24)

The contribution of electrons with momentum \(\hbar k\) to the induced electron density is
\[
n_{\text{ind}}(k, r, t) = \left[ |\psi_k(r, t)|^2 - |\psi_k^{(0)}(r)|^2 \right].
\]  
(29.2.25)

The total induced electron density is obtained by summing over the occupied states
\[
n_{\text{ind}}(r, t) = 2 \sum_{|k| < k_F} \left[ |\psi_k(r, t)|^2 - |\psi_k^{(0)}(r)|^2 \right].
\]  
(29.2.26)

The factor 2 comes from the two spin orientations. Inserting (29.2.24) into this expression, taking into account the normalization factor \(1/\sqrt{V}\) of plane waves and keeping only the terms linear in \(V(q)\), we find
\[
n_{\text{ind}}(r, t) = \frac{2}{V^2} \sum_{|k| < k_F} \left[ \frac{V^*(q)e^{-i(q \cdot r - \omega t)}e^{\delta t}}{\hbar \omega - \varepsilon_{k+q} + \varepsilon_k - i\delta} + \frac{V(q)e^{i(q \cdot r - \omega t)}e^{\delta t}}{-\hbar \omega - \varepsilon_{k-q} + \varepsilon_k + i\delta} + \frac{V(q)e^{i(q \cdot r - \omega t)}e^{\delta t}}{-\hbar \omega - \varepsilon_{k-q} + \varepsilon_k - i\delta} \right].
\]  
(29.2.27)

The Fourier components with both \(q\) and \(-q\) \(|V^*(q) = V(-q)|\) appear in the above expression due to our choice (29.2.18) of the potential. When only the terms proportional to \(V(q)\ \exp(iq \cdot r)\) are collected,
\[
n_{\text{ind}}(r, t) = \frac{2}{V^2} \sum_{|k| < k_F} \left[ \frac{V(q)e^{i(q \cdot r - \omega t)}e^{\delta t}}{-\hbar \omega - \varepsilon_{k-q} + \varepsilon_k - i\delta} + \frac{V(q)e^{i(q \cdot r - \omega t)}e^{\delta t}}{\hbar \omega - \varepsilon_{k+q} + \varepsilon_k + i\delta} \right].
\]  
(29.2.28)
If the summation variable \( k \) is changed in the first term to \( k + q \), the state with \( k + q \) has to be occupied. This condition can be expressed by an appropriately chosen Fermi distribution function. We then get

\[
n_{\text{ind}}(r, t) = \frac{2}{V^2} \sum_k \left[ \frac{f_0(\varepsilon_{k+q})V(q)e^{i(q \cdot r - \omega t)}e^{\delta t}}{-\hbar \omega - \varepsilon_k + \varepsilon_{k+q} - i\delta} \right. \\
+ \left. \frac{f_0(\varepsilon_k)V(q)e^{i(q \cdot r - \omega t)}e^{\delta t}}{\hbar \omega - \varepsilon_{k+q} + \varepsilon_k + i\delta} \right]
\] (29.2.29)

It follows from this expression that the Fourier transform of the induced density is

\[
n_{\text{ind}}(q, \omega) = \frac{2}{V} \sum_k \frac{f_0(\varepsilon_k) - f_0(\varepsilon_{k+q})}{\hbar \omega - \varepsilon_{k+q} + \varepsilon_k + i\delta} V(q).
\] (29.2.30)

Comparison with (29.2.16) gives

\[
\Pi_0(q, \omega) = \frac{2}{V} \sum_k \frac{f_0(\varepsilon_k) - f_0(\varepsilon_{k+q})}{\hbar \omega - \varepsilon_{k+q} + \varepsilon_k + i\delta}.
\] (29.2.31)

Note that the term \( i\delta \) in the denominator originates from the factor \( e^{\delta t} \) describing the adiabatic switching on of the external perturbation, and it ensures the correct analytic properties of \( \Pi_0(q, \omega) \) and of the dielectric function in the complex \( \omega \) plane. By inserting this expression into (29.2.17) we find

\[
\epsilon_r(q, \omega) = 1 - \frac{4\pi e^2}{q^2} \sum_k \frac{f_0(\varepsilon_k) - f_0(\varepsilon_{k+q})}{\hbar \omega - \varepsilon_{k+q} + \varepsilon_k + i\delta}.
\] (29.2.32)

This is known as the Lindhard dielectric function\(^5\) and the response function \( \Pi_0(q, \omega) \) itself is called the Lindhard function.

### 29.2.4 Alternative Derivation of the Lindhard Function

The response function \( \Pi_0 \) of the noninteracting electron system and hence the dielectric function can be calculated even more simply in second quantization. For this we evaluate the spin-resolved generalization of the response function, the quantity \( \Pi_{\sigma\sigma'} \) defined in (29.1.33), for noninteracting electrons.

The first term of the commutator in (29.1.33),

\[
\sum_{kk'} \left\langle c_{k\sigma}^\dagger(t)c_{k+q\sigma}(t)c_{k'\sigma'}^\dagger(t')c_{k'\sigma'}(t') \right\rangle,
\] (29.2.33)

describes the propagation of an electron–hole pair from time \( t' \) when it is created until time \( t \) when the pair is annihilated. Apart from the trivial case

\(^5\) J. Lindhard, 1954.
$q = 0$, the hole with momentum $k'$ and spin $\sigma'$ created at $t'$ has to be filled at $t$ by the electron with momentum $k$ and spin $\sigma$. Hence only the terms with $k' = k$ and $\sigma' = \sigma$ give finite contributions. The electron–hole pair can be created only if the state with wave vector $k$ is occupied in the ground state, while the state with $k + q$ has to be empty. These requirements can be written concisely by the Fermi distribution functions $f_0(\varepsilon_k)$ and $1 - f_0(\varepsilon_{k+q})$. The time dependence of the operators can be evaluated using (28.4.97). Thus we find that

$$\sum_{kk'} \left\langle c_{k\sigma}^\dagger(t)c_{k+q\sigma}(t)c_{k'\sigma'}^\dagger(t')c_{k'\sigma'}(t') \right\rangle = \delta_{\sigma\sigma'} \sum_k e^{i\varepsilon_{k\sigma}(t-t')/\hbar} e^{-i\varepsilon_{k+q\sigma}(t-t')/\hbar} f_0(\varepsilon_k) \left[ 1 - f_0(\varepsilon_{k+q}) \right].$$  \hspace{1cm} (29.2.34)

As a retarded response function (the retardation is ensured by the Heaviside step function) the Fourier transform $\Pi_0(q, \omega)$ with respect to time has to be analytic in the upper complex half-plane. This can be achieved by incorporating a factor $\exp(-\delta|t-t'|)$ with infinitesimal $\delta$, which is equivalent to switching on the perturbation adiabatically. The Fourier transform is then

$$\int_{-\infty}^{\infty} \theta(t-t') e^{i\omega(t-t')} e^{i(\varepsilon_{k\sigma}-\varepsilon_{k+q\sigma})(t-t')/\hbar} e^{-\delta|t-t'|} \text{d}(t-t') = \int_{0}^{\infty} e^{i(h\omega-\varepsilon_{k+q\sigma}+\varepsilon_{k\sigma}+i\delta)(t-t')/\hbar} \text{d}(t-t') \hspace{1cm} (29.2.35)$$

Since the response function is defined in (29.1.33) with a prefactor $-i/\hbar V$, the first term of the commutator yields

$$\frac{1}{V} \delta_{\sigma\sigma'} \sum_k f_0(\varepsilon_k) \left[ 1 - f_0(\varepsilon_{k+q}) \right] \frac{1}{h\omega - \varepsilon_{k+q\sigma} + \varepsilon_{k\sigma} + i\delta}. \hspace{1cm} (29.2.36)$$

Analogously, the second term of the commutator,

$$\sum_{kk'} \left\langle c_{k'\sigma'}^\dagger(t')c_{k'\sigma'}(t')c_{k\sigma}(t)c_{k+q\sigma}(t) \right\rangle, \hspace{1cm} (29.2.37)$$

again gives finite contribution only if $k' = k$ and $\sigma' = \sigma$. However, now the state with quantum number $k$ has to be empty while the state with wave vector $k + q$ has to be occupied. Thus,

$$\sum_{kk'} \left\langle c_{k'\sigma'}^\dagger(t')c_{k'\sigma'}(t')c_{k\sigma}^\dagger(t)c_{k+q\sigma}(t) \right\rangle \hspace{1cm} (29.2.38)$$

$$= \delta_{\sigma\sigma'} \sum_k e^{i\varepsilon_{k+q\sigma}(t'-t)/\hbar} e^{-i\varepsilon_{k\sigma}(t'-t)/\hbar} f_0(\varepsilon_{k+q}) \left[ 1 - f_0(\varepsilon_{k\sigma}) \right].$$
29.2 Dielectric Function of the Uniform Electron Gas

Multiplying it with the step function and incorporating the factor that describes the adiabatic turning on, the Fourier transform of this expression with respect to time gives

\[ \delta_{\sigma\sigma'} \sum_k f_0(\varepsilon_k + q\sigma)[1 - f_0(\varepsilon_{k\sigma})] \frac{i\hbar}{\hbar\omega - \varepsilon_{k+q\sigma} + \varepsilon_{k\sigma} + i\delta}. \]  

(29.2.39)

Multiplying by the prefactor \(-i/\hbar V\) and subtracting the contributions of the two terms of the commutator, we find

\[ \Pi_{0\sigma\sigma'}(q,\omega) = \delta_{\sigma\sigma'} \frac{1}{V} \sum_k \frac{f_0(\varepsilon_{k\sigma}) - f_0(\varepsilon_{k+q\sigma})}{\hbar\omega - \varepsilon_{k+q\sigma} + \varepsilon_{k\sigma} + i\delta}. \]  

(29.2.40)

If the single-particle energies are spin independent, summation over the spin variables gives back the Lindhard function for the polarization bubble

\[ \Pi_0(q,\omega) = 2 \frac{1}{V} \sum_k \frac{f_0(\varepsilon_k) - f_0(\varepsilon_{k+q})}{\hbar\omega - \varepsilon_{k+q} + \varepsilon_k + i\delta}, \]  

(29.2.41)

and the usual form of the Lindhard dielectric function is recovered:

\[ \varepsilon_t(q,\omega) = 1 - \frac{4\pi\tilde{e}^2}{q^2} \frac{2}{V} \sum_k \frac{f_0(\varepsilon_k) - f_0(\varepsilon_{k+q})}{\hbar\omega - \varepsilon_{k+q} + \varepsilon_k + i\delta}. \]  

(29.2.42)

By a change of variables \(k \to -k - q\) in (29.2.39) the second term of the commutator could be written in the form

\[ \delta_{\sigma\sigma'} \sum_k f_0(\varepsilon_{k\sigma})[1 - f_0(\varepsilon_{k+q\sigma})] \frac{i\hbar}{\hbar\omega + \varepsilon_{k+q\sigma} - \varepsilon_{k\sigma} + i\delta}, \]  

(29.2.43)

since the electron energy is an even function of the wave number. Multiplying this expression by \(-i/\hbar V\) and combining it with (29.2.36) the spin-resolved response function can be written as

\[ \Pi_{0\sigma\sigma'}(q,\omega) = \delta_{\sigma\sigma'} \frac{1}{V} \sum_k f_0(\varepsilon_{k\sigma})[1 - f_0(\varepsilon_{k+q\sigma})] \times \left[ \frac{1}{\hbar\omega - \varepsilon_{k+q\sigma} + \varepsilon_{k\sigma} + i\delta} - \frac{1}{\hbar\omega + \varepsilon_{k+q\sigma} - \varepsilon_{k\sigma} + i\delta} \right]. \]  

(29.2.44)

The term that contains the product of the two Fermi distribution functions gives vanishing contribution. This can again be shown by a change of variables \(k \to -k - q\). While the product of the Fermi distribution functions remains unchanged, the expression in the square bracket changes sign; thus, there is complete cancelation when the sum over \(k\) is performed and the expression then simplifies to
\[ \Pi_{0\sigma\sigma'}(q,\omega) = \delta_{\sigma\sigma'} \frac{1}{V} \sum_k f_0(\varepsilon_{k\sigma}) \times \left[ \frac{1}{\hbar \omega - \varepsilon_{k+q\sigma} + \varepsilon_{k\sigma} + i\delta} - \frac{1}{\hbar \omega + \varepsilon_{k+q\sigma} - \varepsilon_{k\sigma} + i\delta} \right], \] 

while the Lindhard dielectric function can be written as 

\[ \epsilon_r(q,\omega) = 1 - \frac{4\pi e^2}{q^2} \frac{2}{V} \sum_k f_0(\varepsilon_k) \times \left[ \frac{1}{\hbar \omega - \varepsilon_{k+q} + \varepsilon_k + i\delta} - \frac{1}{\hbar \omega + \varepsilon_{k+q} - \varepsilon_k + i\delta} \right]. \] 

### 29.2.5 Explicit Form of the Lindhard Dielectric Function

The dielectric function \( \epsilon_r(q,\omega) \) can be decomposed into real and imaginary parts:

\[ \epsilon_r(q,\omega) = \epsilon_1(q,\omega) + i \epsilon_2(q,\omega). \] 

Taking the expression given in (29.2.42) and using (C.3.3) we find

\[ \epsilon_1(q,\omega) = 1 - \frac{4\pi e^2}{q^2} \frac{2}{V} \sum_k f_0(\varepsilon) - \frac{f_0(\varepsilon_{k+q})}{\hbar \omega - \varepsilon_{k+q} + \varepsilon_k} \] 

and

\[ \epsilon_2(q,\omega) = \frac{4\pi e^2}{q^2} \frac{2}{V} \sum_k [f_0(\varepsilon_k) - f_0(\varepsilon_{k+q})] \delta(\hbar \omega - \varepsilon_{k+q} + \varepsilon_k). \]

On the other hand, if the form given in (29.2.46) is used, we obtain

\[ \epsilon_1(q,\omega) = 1 - \frac{4\pi e^2}{q^2} \frac{2}{V} \sum_k f_0(\varepsilon_k) \times \left[ \frac{1}{\hbar \omega - (\varepsilon_{k+q} - \varepsilon_k)} - \frac{1}{\hbar \omega + (\varepsilon_{k+q} - \varepsilon_k)} \right] \] 

and

\[ \epsilon_2(q,\omega) = \frac{4\pi e^2}{q^2} \frac{2}{V} \sum_k f_0(\varepsilon_k) \left[ \delta(\hbar \omega - \varepsilon_{k+q} + \varepsilon_k) - \delta(\hbar \omega - \varepsilon_k + \varepsilon_{k+q}) \right]. \]

It is readily seen from these expressions that the real part of the dielectric function is even in \( \omega \), while the imaginary part is an odd function of \( \omega \).

The summation can be performed exactly in both the real and the imaginary parts at temperature \( T = 0 \) if it is transformed into an integral in \( k \)-space. Using (29.2.50) for the real part and integrating first over the angle \( \theta \) between \( k \) and \( q \) and then over the length of \( k \), we find
Dielectric Function of the Uniform Electron Gas

\( \epsilon_1(q, \omega) = 1 + \frac{q_{TF}^2}{q^2} \left\{ \frac{1}{2} + \frac{k_F}{4q} \left[ 1 - \left( \frac{\hbar \omega + \epsilon_q}{\hbar v_F q} \right)^2 \right] \ln \left( \frac{\hbar \omega + \hbar v_F q + \epsilon_q}{\hbar \omega - \hbar v_F q + \epsilon_q} \right) \right\} \)

with \( \epsilon_q = \hbar^2 q^2 / 2m_e \), and \( q_{TF} \) is the Thomas–Fermi wave number defined in (29.2.13).

In the static case the dielectric function simplifies to

\( \epsilon_r(q) = 1 + \frac{q_{TF}^2}{q^2} \left[ \frac{1}{2} + \frac{k_F}{2q} \left( 1 - \frac{q^2}{4k_F^2} \right) \ln \left| \frac{q + 2k_F}{q - 2k_F} \right| \right] \).

For later convenience this is written in the form

\( \epsilon_r(q) = 1 + \frac{q_{TF}^2}{q^2} F(q/2k_F) = 1 + \frac{4\pi e^2}{q^2} \rho(\epsilon_F) F(q/2k_F) \),

where the function \( F(x) \) is defined in (28.3.85). Here it appears with the argument \( x = q/2k_F \). Making use of the fact that \( F(x) \approx 1 \) for small values of \( x \), as can be seen in Fig. 28.4, the result of the Thomas–Fermi approximation is recovered in the long-wavelength limit. This is not surprising since we know that the Thomas–Fermi approximation is applicable for spatially slowly varying potentials. Recalling that the derivative of \( F(x) \) is logarithmically singular at \( x = 1 \), it follows that the derivative of the dielectric function is also logarithmically singular at \( q = 2k_F \). This has – as will be seen – serious implications. Among others this gives rise to the Friedel oscillations of the screening charge.

According to (29.2.49) the imaginary part is finite only at those \( \omega \) values for which \( \hbar \omega \) is equal to the excitation energy of an electron–hole pair, i.e.,

\( \hbar \omega = \epsilon_{k+q} - \epsilon_k = \frac{\hbar^2 q^2}{m_e} \cdot k + \frac{\hbar^2 q^2}{2m_e} \).

This is quite natural since the imaginary part is related to the energy dissipation and the electron system can absorb energy from the external field through electron–hole pair excitations. We saw already in Fig. 28.9 that these excitations form a broad continuum. Knowing that \( \epsilon_2(q, \omega) \) is an odd function of \( \omega \), we list the results for \( \omega > 0 \) only. One has to distinguish three frequency ranges. For \( q < 2k_F \)

\( \epsilon_2(q, \omega) = \begin{cases} \frac{\pi \hbar \omega}{2 \hbar v_F q} \frac{q_{TF}^2}{q^2} & 0 \leq \hbar \omega < \hbar v_F q - \epsilon_q, \\ \frac{\pi k_F}{4 q} \left[ 1 - \left( \frac{\hbar \omega - \epsilon_q}{\hbar v_F q} \right)^2 \right] \frac{q_{TF}^2}{q^2} & \hbar v_F q - \epsilon_q \leq \hbar \omega \leq \hbar v_F q + \epsilon_q, \\ 0 & \hbar v_F q + \epsilon_q \leq \hbar \omega, \end{cases} \)

(29.2.56)
while for \( q > 2k_F \)

\[
\epsilon_2(q, \omega) = \begin{cases} 
0 & 0 \leq \hbar \omega < \varepsilon_q - \hbar v_F q, \\
\frac{\pi k_F}{4q} \left[ 1 - \left( \frac{\hbar \omega - \varepsilon_q}{\hbar v_F q} \right)^2 \right] \frac{q_T^2}{q^2} & \varepsilon_q - \hbar v_F q \leq \hbar \omega \leq \varepsilon_q + \hbar v_F q, \\
0 & \varepsilon_q + \hbar v_F q \leq \hbar \omega.
\end{cases}
\]

(29.2.57)

Figure 29.7 shows the frequency dependence of the real and imaginary parts of the dielectric function for positive \( \omega \) for small, intermediate, and large values of \( q/k_F \).

![Figure 29.7](image)

**Fig. 29.7.** Frequency dependence of the real and imaginary parts of the dielectric function of the electron gas for small, intermediate, and large values of the wave number. The results are shown for a typical metallic electron density, \( r_s = 3 \)

As a retarded function, \( \Pi(q, \omega) \) is analytic in the upper half-plane. Hence, it has to satisfy the Kramers–Kronig relations given in (J.1.70):

\[
\text{Re} \left\{ \frac{1}{\varepsilon_r(q, \omega)} \right\} - 1 = \frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \text{Im} \left\{ \frac{1}{\varepsilon_r(q, \omega')} \right\} \frac{1}{\omega' - \omega} \quad (29.2.58)
\]

and

\[
\text{Im} \left\{ \frac{1}{\varepsilon_r(q, \omega)} \right\} = \frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \left[ 1 - \text{Re} \left\{ \frac{1}{\varepsilon_r(q, \omega')} \right\} \right] \frac{1}{\omega' - \omega}. \quad (29.2.59)
\]

We also note that since the dielectric function establishes a causal relationship between the electric displacement and the electric field, the Kramers–
Kronig relations are valid between the real and imaginary parts of the dielectric function as well. These relations were given in (16.1.65).

### 29.2.6 Corrections Beyond the RPA

If we wish to go beyond the RPA, the methods of many-body theory have to be used. There are several possibilities for that. One of them is to calculate $\tilde{\Pi}(q,\omega)$ up to a given order of perturbation theory. Another is to select an infinite set of irreducible diagrams for the two-particle Green function according to some physical considerations and to sum up their contributions. For this let us notice that there is a large class of processes in which the electron and the hole of the pair propagate independently of one another in the sense that although they interact with the other electrons of the Fermi sea, there are no intermediate scattering processes that would couple the electron to the hole either directly or indirectly. Such processes are displayed in Fig. 29.8.

![Fig. 29.8. Scattering processes during the propagation of the electron–hole pair that lead to the renormalization of the energy of the electron and the hole separately](image)

These processes have a simple physical interpretation: the electron and the hole propagating in the system are not bare particles but quasiparticles. Their energy is not $\varepsilon_{k+q}$ and $\varepsilon_k$, respectively; it is renormalized by the interaction with the rest of the electron system. The first two diagrams correspond to the simplest Hartree and Fock corrections to the energy, but higher order processes should also be taken into account. When only such self-energy corrections are considered, the dielectric function still has a Lindhard-like form; however the energy of quasiparticles $\tilde{\varepsilon}_k$ appears in place of $\varepsilon_k$, the energy of free electrons. We then have

$$\epsilon_r(q,\omega) = 1 - \frac{4\pi\varepsilon^2}{q^2} \frac{2}{V} \sum_k \frac{f_0(\tilde{\varepsilon}_k) - f_0(\tilde{\varepsilon}_{k+q})}{\hbar\omega - \tilde{\varepsilon}_{k+q} + \tilde{\varepsilon}_k + i\delta}.$$  \hspace{1cm} (29.2.60)

This approximation is called the renormalized RPA.
A further possibility is to use the equation-of-motion method explained briefly in Appendix J. That method relies on solving the equation of motion

$$\frac{dn(q,t)}{dt} = \frac{i}{\hbar} [\mathcal{H}, n(q,t)]$$

(29.2.61)

for the Fourier transform of the operator of electron density given in second-quantized form in (28.4.96), where $\mathcal{H}$ denotes the total Hamiltonian of the system that includes, besides the kinetic energy and the interaction given in (28.1.34), the external potential $V_{\text{ext}}(r,t)$. This last term, which is treated as a perturbation, is used in one of the equivalent forms. It is written either in real space in terms of the field operators or in momentum space in terms of the Fourier transforms of the potential and density. The Fourier transform of the density can also be expressed in terms of the creation and annihilation operators. Thus we have

$$\mathcal{H}_1(t) = \sum_\sigma \int \hat{\psi}_\sigma^\dagger(r) V_{\text{ext}}(r,t) \hat{\psi}_\sigma(r) \, dr$$

$$= \frac{1}{V} \sum_q V_{\text{ext}}(q,t) n(-q)$$

(29.2.62)

Once the equation of motion is solved for $n(q,t)$, the induced charge is its expectation value:

$$n_{\text{ind}}(q,t) = \langle n(q,t) \rangle.$$  

(29.2.63)

As known from our earlier calculations, and it follows also from the derivation given in Appendix J, in a noninteracting system the electron density induced by the external potential is

$$n_{\text{ind}}(q,\omega) = \Pi_0(q,\omega) V_{\text{ext}}(q,\omega)$$

(29.2.64)

with the known $\Pi_0$. If the external potential is generated by an external charge,

$$n_{\text{ind}}(q,\omega) = \Pi_0(q,\omega) \frac{4\pi\tilde{e}^2}{q^2} n_{\text{ext}}(q,\omega).$$

(29.2.65)

New, more complicated terms appear on the right-hand side of the equation of motion when the electron–electron interaction is taken into account. Depending on the treatment of these terms different approximation schemes are obtained; some details of which can be found in Appendix J. Here we present only the results, motivating them by using a simple approach.

If the interacting electron system is treated in the RPA,

$$n_{\text{ind}}(q,\omega) = \frac{\Pi_0(q,\omega)}{1 - (4\pi\tilde{e}^2/q^2)\Pi_0(q,\omega)} V_{\text{ext}}(q,\omega) = \Pi_0(q,\omega) V(q,\omega),$$

(29.2.66)
where \( V(q, \omega) = V_{\text{ext}}(q, \omega)/\epsilon_r(q, \omega) \) is the screened potential. Combining this expression with the first equation of (29.1.22) we have

\[
n_{\text{ind}}(q, \omega) = \Pi_0(q, \omega) \frac{4\pi \tilde{e}^2}{q^2} n(q, \omega) = \Pi_0(q, \omega) \frac{4\pi \tilde{e}^2}{q^2} [n_{\text{ext}}(q, \omega) + n_{\text{ind}}(q, \omega)].
\]  

(29.2.67)

This expression is similar to (29.2.65) which is valid for noninteracting electrons except that the induced electron density is found to be proportional to the total density. We know that owing to exchange and correlations, electrons repel other electrons from their close vicinity creating Fermi and Coulomb holes around themselves. Therefore, a presumably better approximation can be achieved by assuming that the electron system does not react to the full charge, but to a charge corrected by the local field. If so, then only an effective particle density

\[
n_{\text{eff}}(q, \omega) = n_{\text{ext}}(q, \omega) + [1 - G(q)] n_{\text{ind}}(q, \omega)
\]  

(29.2.68)

should appear on the right-hand side of (29.2.67). The quantity \( G(q) \) is the so-called local-field factor and accounts for the short-range exchange and correlation effects not present in the RPA. With this assumption the dielectric function takes the form

\[
\frac{1}{\epsilon_r(q, \omega)} = 1 + \frac{4\pi \tilde{e}^2}{q^2} \frac{\Pi_0(q, \omega)}{1 - (4\pi \tilde{e}^2/q^2) [1 - G(q)] \Pi_0(q, \omega)}.
\]  

(29.2.69)

This expression shows that \( G(q) \) weakens the screening.

The local-field factor has to be determined using physical considerations. Depending on its choice different approximation schemes are obtained. Using the equation-of-motion method for the screening charge, as explained in Appendix J, J. Hubbard (1957) proposed the expression

\[
G(q) = \frac{1}{2} \frac{q^2}{q^2 + k_F^2}.
\]  

(29.2.70)

Somewhat later K. S. Singwi and A. Sjölander (1967) have shown that a better approximation can be achieved if \( G(q) \) is chosen in the form

\[
G(q) = q \int_0^\infty dr \ [1 - g(r)] j_1(qr),
\]  

(29.2.71)

where \( g(r) \) is the pair distribution function and \( j_1 \) is the first-order spherical Bessel function. The RPA corresponds to completely neglecting this local-field correction.
29.2.7 Effect of Finite Relaxation Time

Until now the electron states have been assumed to have infinite lifetime. Although the states near the Fermi energy have a rather long lifetime if only the electron–electron interaction is taken into account, impurities that are unavoidably present in the sample or interaction with phonons can give rise to a substantial shortening of the lifetime. Here, we will consider the effect of the finite lifetime on the dielectric function in the semiclassical approximation. The induced charge will be determined using the nonstationary Boltzmann equation in an improved relaxation-time approximation.

We assume a space- and time-dependent external perturbation described by a periodically varying scalar potential

$$\varphi(r, t) = \varphi(q)e^{i(q \cdot r - \omega t)}.$$  \hspace{1cm} (29.2.72)

The force acting on the electron is

$$F = -eE = e \text{grad} \varphi(r) = ieq\varphi(q)e^{i(q \cdot r - \omega t)},$$  \hspace{1cm} (29.2.73)

or, when expressed in terms of $V(q) = -e\varphi(q)$,

$$F = -iqV(q)e^{i(q \cdot r - \omega t)}.\hspace{1cm} (29.2.74)$$

This perturbation gives rise to a periodically varying term in the distribution function which can be written as

$$f(k, r, t) = f_0(n_0) + f_1(k)e^{i(q \cdot r - \omega t)},$$  \hspace{1cm} (29.2.75)

where $f_0(n_0)$ is the distribution function corresponding to the uniform charge density $n_0$. However, when the effect of collisions is treated in the relaxation-time approximation of the Boltzmann equation, we should take into account that the electron density relaxes to its local equilibrium value $n(r, t)$ and not to its uniform equilibrium value $n_0$. Thus, when the explicit time dependence of the distribution function is kept in the Boltzmann equation [see (24.2.16)] and this improved relaxation-time approximation is used for the collision integral, we have

$$\frac{\partial f}{\partial t} + v_k \frac{\partial f}{\partial r} + \frac{1}{\hbar} F(r, t) \frac{\partial f}{\partial k} = -\frac{f - f_0[n(r, t)]}{\tau}.\hspace{1cm} (29.2.76)$$

If the difference between distribution functions belonging to the local equilibrium density and the uniform density is denoted by

$$\delta_n f_0 = f_0(n) - f_0(n_0),\hspace{1cm} (29.2.77)$$

the Boltzmann equation linearized in $f_1$ takes the form

$$\frac{\partial f_1}{\partial t} + v_k \frac{\partial f_1}{\partial r} + \frac{1}{\hbar} F(r, t) \frac{\partial f_0}{\partial k} = -\frac{f_1}{\tau} + \frac{\delta_n f_0}{\tau}.\hspace{1cm} (29.2.78)$$
The equilibrium distribution function \( f_0 \) depends on \( k \) through the energy only. Making use of the periodic spatial and temporal variation of the distribution function and using (29.2.74) for the force we have

\[
- \imath \omega f_1 + \imath q \cdot v_k f_1 - \imath q \cdot v_k V(q) \frac{\partial f_0}{\partial \varepsilon} = - \frac{f_1}{\tau} + \frac{\delta_n f_0}{\tau} .
\] (29.2.79)

The formal solution of this equation yields

\[
f_1 = \frac{\imath q \cdot v_k \tau V(q) \frac{\partial f_0}{\partial \varepsilon} + \delta_n f_0}{1 - \imath \omega \tau + \imath q \cdot v_k \tau} .
\] (29.2.80)

The induced number density is obtained by summing the contributions of all occupied states, that is by summing \( f_1 \) over the \( k \) vectors within the Fermi sphere:

\[
n_{\text{ind}} = \frac{2}{V} \sum_{|k| < k_F} f_1(k) .
\] (29.2.81)

The distribution function changes significantly, however, only in the neighborhood of the Fermi energy. This is seen when the second term in the numerator of (29.2.80) is rewritten using the expansion

\[
\delta_n f_0 = f_0(n) - f_0(n_0) = \frac{\partial f_0}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial n} \delta n ,
\] (29.2.82)

where \( \delta n \) is the induced particle density. We know from the Thomas–Fermi approximation that for long-wavelength disturbances

\[
\frac{\partial n}{\partial \varepsilon} = - \rho(\varepsilon_F) ,
\] (29.2.83)

and thus

\[
\delta_n f_0 = - \frac{1}{\rho(\varepsilon_F)} \frac{\partial f_0}{\partial \varepsilon} n_{\text{ind}} .
\] (29.2.84)

Averaging first over the angle between \( q \) and \( v_k \) on the Fermi surface yields

\[
\langle f_1 \rangle_{\text{ave}} = V(q) \frac{\partial f_0(k)}{\partial \varepsilon} \left[ 1 + \frac{\omega + \imath \tau}{2 \nu_F q} \ln \left( \frac{\omega - \nu_F q + \imath \tau}{\omega - \nu_F q + \imath \tau} \right) \right]
- \frac{n_{\text{ind}}}{\rho(\varepsilon_F)} \frac{\partial f_0(k)}{\partial \varepsilon} \frac{1}{2 \nu_F q \tau} \ln \left( \frac{\omega - \nu_F q + \imath \tau}{\omega + \nu_F q + \imath \tau} \right) .
\] (29.2.85)

Then the integral over the length of \( k \) is performed by converting it to an integral over energy. It is readily obtained that

\[
n_{\text{ind}} = - V(q) \rho(\varepsilon_F) \left[ 1 + \frac{\omega + \imath \tau}{2 \nu_F q} \ln \left( \frac{\omega - \nu_F q + \imath \tau}{\omega + \nu_F q + \imath \tau} \right) \right]
+ \frac{n_{\text{ind}}}{2 \nu_F q \tau} \ln \left( \frac{\omega - \nu_F q + \imath \tau}{\omega + \nu_F q + \imath \tau} \right) .
\] (29.2.86)
The solution of this equation for $n_{\text{ind}}$ leads to the following expression for the response function $\tilde{\Pi}$:

$$\tilde{\Pi}(q, \omega) = -\rho(\varepsilon_F) \frac{1 + \frac{\omega + i/\tau}{2v_F q} \ln \left( \frac{\omega - v_F q + i/\tau}{\omega + v_F q + i/\tau} \right)}{1 + \frac{i/\tau}{2v_F q} \ln \left( \frac{\omega - v_F q + i/\tau}{\omega + v_F q + i/\tau} \right)}.$$  \hspace{1cm} (29.2.87)

The dielectric function then takes the form

$$\epsilon_T(q, \omega) = 1 + \frac{4\pi \tilde{e}^2}{q^2} \rho(\varepsilon_F) \frac{1 + \frac{\omega + i/\tau}{2v_F q} \ln \left( \frac{\omega - v_F q + i/\tau}{\omega + v_F q + i/\tau} \right)}{1 + \frac{i/\tau}{2v_F q} \ln \left( \frac{\omega - v_F q + i/\tau}{\omega + v_F q + i/\tau} \right)}.$$  \hspace{1cm} (29.2.88)

In the static, $\omega \to 0$ limit the semiclassical Thomas–Fermi result is recovered, while in the long-wavelength, $q \to 0$ limit we find

$$\tilde{\Pi}(q, \omega) = \frac{n_e q^2}{m_e \omega (\omega + i/\tau)},$$  \hspace{1cm} (29.2.89)

where $n_e = k_F^3/3\pi^2$ is the electron density. It then follows that

$$\epsilon_T(\omega) = 1 - \frac{4\pi n_e \tilde{e}^2}{m_e \omega (\omega + i/\tau)}.$$  \hspace{1cm} (29.2.90)

This expression is identical to the result derived for the frequency-dependent dielectric function in the Drude model [see (16.1.68)]. This has been used in Chapter 25 to study the optical properties of metals. To get a more accurate expression with a better $q$ dependence than the Thomas–Fermi result, a quantum mechanical treatment is needed. We note that the naive approximation in which the polarization bubble of the RPA is calculated for an electron and a hole with finite lifetime $\tau$ would yield a Lindhard-like expression where $\omega + i\delta$ is replaced with $\omega + i/\tau$, i.e.,

$$\tilde{\Pi}(q, \omega) = \Pi_0(q, \omega + i/\tau) = \frac{2}{V} \sum_k \frac{f_0(\varepsilon_k) - f_0(\varepsilon_{k+q})}{\hbar \omega - \varepsilon_{k+q} - \varepsilon_k + i/\tau}.$$  \hspace{1cm} (29.2.91)

We know from our earlier considerations that this approach does not give a physically correct result since in a periodically driven system relaxation is toward local equilibrium and not toward thermodynamic equilibrium. When this is taken into account, one finds the so-called Lindhard–Mermin\(^6\) form for the dielectric function

$$\epsilon_T(q, \omega) = 1 - \frac{4\pi \tilde{e}^2}{q^2} \frac{\left[ 1 + i/(\omega \tau) \right] \Pi_0(q, \omega + i/\tau)}{1 + i/(\omega \tau) \left[ \Pi_0(q, \omega + i/\tau)/\Pi_0(q, 0) \right]}.$$  \hspace{1cm} (29.2.92)

In the $\tau \to \infty$ limit the Lindhard form of the dielectric function (29.2.32) is recovered. This expression also yields the correct static limit and the known expression for the frequency-dependent conductivity.

\(^6\) N. D. Mermin, 1970.
29.3 Static Screening

One essential feature of the above-derived result for the dielectric function is its $1/q^2$ divergence in the long-wavelength ($q \to 0$) limit. As a consequence of that, the electronic charge distribution is drastically modified if an external charge is introduced into a simple metal. We show below that the induced charge screens completely the external charge.

The potential created by a pointlike external charge $Q$ is

$$\varphi_{\text{ext}}(r) = \frac{Q}{4\pi \epsilon_0 r}.$$  \hspace{1cm} (29.3.1)

Equation (C.1.63) implies that the Fourier transform of the potential is

$$\varphi_{\text{ext}}(q) = \frac{Q}{\epsilon_0 q^2}.$$  \hspace{1cm} (29.3.2)

This potential gives rise to an inhomogeneous charge distribution in the vicinity of the external charge. In the static case, the Fourier transform of the induced number density is given according to (29.1.24) by

$$n_{\text{ind}}(q) = \Pi(q) V_{\text{ext}}(q) = -e \Pi(q) \varphi_{\text{ext}}(q) = -\frac{eQ}{\epsilon_0 q^2} \Pi(q).$$  \hspace{1cm} (29.3.3)

If the density–density response function is expressed in terms of the dielectric function using (29.1.25) we get

$$n_{\text{ind}}(q) = \frac{Q}{e} \left[ 1 - \frac{1}{\epsilon_r(q)} \right]$$  \hspace{1cm} (29.3.4)

or, if the irreducible polarization function is used,

$$n_{\text{ind}}(q) = -\frac{eQ}{\epsilon_0 q^2} \frac{\tilde{\Pi}(q)}{1 - \frac{e^2}{\epsilon_0 q^2} \tilde{\Pi}(q)}.$$  \hspace{1cm} (29.3.5)

The total induced charge, the volume integral of the induced charge density $\rho_{\text{ind}}(r) = -en_{\text{ind}}(r)$, is equal to the $q = 0$ Fourier component of the induced charge density. If $\tilde{\Pi}(q)$ remains finite in the limit $q \to 0$, which is the case in the homogeneous electron gas and in metals as well,

$$Q_{\text{ind}} = -e \lim_{q \to 0} n_{\text{ind}}(q) = Q \lim_{q \to 0} -\frac{eQ}{\epsilon_0 q^2} \frac{\tilde{\Pi}(q)}{1 - \frac{e^2}{\epsilon_0 q^2} \tilde{\Pi}(q)} = -Q.$$  \hspace{1cm} (29.3.6)

The sign of the total induced charge is opposite to that of the external charge and they are equal in magnitude; hence, screening is indeed complete in
metals. In semiconductors, where there are mobile carriers, but $\tilde{\Pi}(q)$ vanishes at $q = 0$ owing to the absence of low-energy electron–hole pair excitations, screening is not complete.

In what follows we will show, calculating the spatial variation of the screening charge and the screened potential, that in metals, where screening is complete, screening of the long-range Coulomb potential leads to a short-range effective interaction.

### 29.3.1 Thomas–Fermi Screening

It follows from (29.1.16) that the Fourier transform of the screened potential around a charge $Q$ introduced into a metal is

$$\varphi(q) = \frac{1}{\epsilon_{t}(q)} \varphi_{\text{ext}}(q) = \frac{1}{\epsilon_{t}(q)} \frac{Q}{\epsilon_{0} q^{2}}. \quad (29.3.7)$$

The Thomas–Fermi approximation for the dielectric function [see (29.2.12)] gives

$$\varphi(q) = \frac{Q}{\epsilon_{0}(q^{2} + q_{\text{TF}}^{2})}, \quad (29.3.8)$$

which shows that the $1/q^{2}$ singularity of the Coulomb potential is removed by the screening effect of the electrons.

The spatial variation of the screened potential can be obtained by taking the inverse Fourier transform. According to (C.1.62)

$$\varphi(r) = \frac{1}{V} \sum_{q} \frac{Q}{\epsilon_{0}(q^{2} + q_{\text{TF}}^{2})} e^{i \mathbf{q} \cdot \mathbf{r}} = \frac{Q}{4 \pi \epsilon_{0} r} e^{-q_{\text{TF}} r}. \quad (29.3.9)$$

This is the well-known Yukawa potential of nuclear physics. The spatial variation of the induced charge is given according to (29.2.6) by

$$\rho_{\text{ind}}(r) = -en_{\text{ind}}(r) = -e^{2} \rho(\varepsilon_{F}) \varphi(r) = -e^{2} \rho(\varepsilon_{F}) \frac{Q}{4 \pi \epsilon_{0} r} e^{-q_{\text{TF}} r}. \quad (29.3.10)$$

If the prefactor is expressed in terms of the Thomas–Fermi wave number, we find

$$\rho_{\text{ind}}(r) = -\frac{Q}{4 \pi} \frac{q_{\text{TF}}^{2}}{r} e^{-q_{\text{TF}} r}. \quad (29.3.11)$$

The total induced charge is its volume integral

$$Q_{\text{ind}} = \int_{V} \rho_{\text{ind}}(r) \, dr = -\frac{Q}{4 \pi} \int_{0}^{\infty} \frac{q_{\text{TF}}^{2}}{r} e^{-q_{\text{TF}} r} 4 \pi r^{2} \, dr$$

$$= -Q \int_{0}^{\infty} xe^{-x} \, dx = -Q, \quad (29.3.12)$$
as has already been demonstrated generally. The redistribution of the electric charge is so drastic that the screened potential decreases exponentially fast. The characteristic screening length is \( 1/q_{TF} \); the external charge is practically not felt at distances larger than a few times \( 1/q_{TF} \).

Before estimating the screening length for metals we note that this type of exponential screening of external charges is well known in the Debye–Hückel theory of electrolytes, which are classical, nondegenerate charged systems, but their screening length is essentially different from that in degenerate systems. According to the classical Maxwell–Boltzmann distribution applicable to electrolytes and also to nondegenerate semiconductors, the density of particles varies as

\[
\rho_n(r) = n_e e^{-V(r)/k_B T} \tag{29.3.13}
\]

when the energy is changed locally by an amount \( V(r) \). This expression can be expanded to linear order if the potential is weak, and the change in the particle density is given by

\[
\rho_{ind}(r) = -\frac{n_e}{k_B T} V(r). \tag{29.3.14}
\]

Comparison of this expression with (29.2.6) shows that the response of classical particles is given by \( n_e/k_B T \) instead of the density of states \( \rho(\varepsilon_F) \). Using this in the dielectric function an expression similar to the Thomas–Fermi approximation is obtained, where screening is characterized by the Debye–Hückel wave number defined via

\[
q_{DH}^2 = \frac{n_e e^2}{\epsilon_0 k_B T} = \frac{4\pi n_e e^2}{k_B T}. \tag{29.3.15}
\]

The inverse of this wave number is the Debye length which was introduced and used already in Chapter 27 where the properties of semiconductors were studied.

For the degenerate electron gas, where the Fermi distribution function applies, the density of states of the three-dimensional free electron gas is used in (29.2.13) to estimate the screening length. Comparing \( q_{TF} \) to the Fermi momentum and expressing \( k_F \) with the radius \( r_0 \) of the Wigner–Seitz sphere available for an electron or with the dimensionless \( r_s \), we find

\[
\frac{q_{TF}^2}{k_F^2} = \frac{4\pi e^2 m_e k_F}{\hbar^2 \pi^2} = \left( \frac{16}{3\pi^2} \right)^{2/3} \frac{r_0}{a_0} = \left( \frac{16}{3\pi^2} \right)^{2/3} r_s, \tag{29.3.16}
\]

from which

\[
q_{TF} = 0.815 k_F r_s^{1/2}. \tag{29.3.17}
\]

The typical range for \( r_s \) is between 1.8 and 6 in metals. This implies that \( q_{TF} \) is of the same order as \( k_F \). Since the inverse of \( k_F \) is on the order of atomic distances, screening occurs on the same length scale in metals.
29.3.2 Friedel Oscillations

The Thomas–Fermi approximation gives only a crude picture of the spatial variation of the screening charge since screening occurs on the atomic scale while the approximation is applicable for long-wavelength variations only. We have therefore to consider how the result changes when the Lindhard function with its correct $q$ dependence is used for $\Pi_0$ and not its $q \to 0$ limit.

For that one would have to repeat the calculation of the induced charge by inserting the Lindhard form of the dielectric function into (29.3.4), and then taking the inverse Fourier transform of $n_{\text{ind}}(q)$. Unfortunately, this inverse Fourier transform cannot be calculated exactly. Therefore, we apply a different procedure used already in Chapter 16 when we studied the scattering of electrons by an impurity. Equation (16.4.44) shows already that at distances far from the impurity, outside the range of the atomic potential, the induced density decays as $1/r^3$ and it is modulated by an oscillatory function. These oscillations will be discussed further here.

When the incoming particle is described by a plane wave and the scattering center by a potential $V(r)$, it follows from (16.4.4) that the wavefunction satisfies the equation

$$
\psi_k(r) = \frac{1}{\sqrt{V}} e^{ik \cdot r} + \int dr' G(r - r') V(r') \psi_k(r'),
$$

(29.3.18)

where

$$
G(r - r') = -\frac{m_e e^{i|\mathbf{r} - \mathbf{r}'|}}{2\pi \hbar^2 |\mathbf{r} - \mathbf{r}'|}
$$

(29.3.19)

is the Green function of free electrons. The first iteration gives

$$
\psi_k(r) = \frac{1}{\sqrt{V}} e^{ik \cdot r} \left[ 1 + \int dr' G(r - r') V(r') e^{ik \cdot (r' - r)} \right].
$$

(29.3.20)

When the change in the electron density is calculated from this expression up to first order in the potential, we get

$$
n_{\text{ind}}(r) = \frac{2}{V} \sum_{|k| < k_F} \int dr' V(r')
$$

(29.3.21)

$$
\times \left[ G(r - r') e^{ik \cdot (r' - r)} + G^*(r - r') e^{-ik \cdot (r' - r)} \right],
$$

where the factor 2 comes from the two spin orientations. Using (29.3.19) for the Green function, replacing the sum by an integral, and performing first the integration over the angular variable, we have

$$
n_{\text{ind}}(r) = -\frac{m_e}{2\pi^3 \hbar^2} \int dr' V(r') \int_0^{k_F} dk \ k^2 \left[ \frac{\sin k |\mathbf{r} - \mathbf{r}'|}{k |\mathbf{r} - \mathbf{r}'|} \cdot \frac{2 \cos k |\mathbf{r} - \mathbf{r}'|}{|\mathbf{r} - \mathbf{r}'|} \right].
$$

(29.3.22)
Performing then the integral over $k$ gives

$$n_{\text{ind}}(r) = \frac{2m_ek_F^4}{\pi^3\hbar^2} \int dr' V(r') g(2k_F|r-r'|), \quad (29.3.23)$$

where

$$g(x) = \frac{x \cos x - \sin x}{x^4}. \quad (29.3.24)$$

If the potential $V(r)$ varies slowly in space compared to the inverse of $2k_F$ over which this oscillatory function decays, then the local relationship (29.2.6) found in the Thomas–Fermi approximation holds true between the induced charge density and the perturbing potential. If, on the other hand, the screened potential is short ranged, as is the case in metals, then asymptotically, beyond the screening length, the induced charge density decays as

$$n_{\text{ind}}(r) \sim \cos \frac{2k_Fr}{(2k_F)^3}, \quad (29.3.25)$$

as has already been seen in (16.4.44). This slowly decaying oscillation is the consequence of the weak (logarithmic) singularity in the derivative of the Lindhard function at $q = 2k_F$. Physically it is due to the sharp Fermi edge in the momentum distribution of electrons. The wavelength of the oscillation is determined by $1/2k_F$.

It can be shown using a somewhat more rigorous calculation that asymptotically, far from the impurity, only the $q = 2k_F$ Fourier components of the bare external potential $V_{\text{ext}} = -e\varphi_{\text{ext}}$ and of the dielectric function play a role, and the induced charge density is given by the expression

$$\rho_{\text{ind}}(r) \approx -\frac{e^2}{4\pi} \rho(\varepsilon_F) \frac{\varphi_{\text{ext}}(2k_F)}{\varepsilon_r^2(2k_F)} \frac{\cos 2k_Fr}{r^3}. \quad (29.3.26)$$

It is interesting to note that the induced charge is not proportional to the $2k_F$ Fourier component of the screened potential; the square of the dielectric function appears in the denominator. Inserting the Fourier transform of the Coulomb potential of the localized charge $Q$ and using the Lindhard function, we find

$$\rho_{\text{ind}}(r) \approx -\frac{Q}{4\pi} \frac{\xi^2}{(1 + \xi^2/2)^2} \frac{\cos 2k_Fr}{r^3} \quad (29.3.27)$$

with $\xi = q_{\text{TF}}/2k_F$.

### 29.4 Dielectric Function of Metals and Semiconductors

In the foregoing, the Lindhard function and the dielectric function have been calculated for electrons moving in a uniform background. Plane-wave wavefunctions and a quadratic dispersion relation have been assumed. The result
obtained may be valid for simple metals where the contribution of the fully occupied bands lying deep below and the completely empty bands lying far above the Fermi energy can be neglected, and the main contribution to the dielectric function comes from electrons of a single partially filled conduction band. If the states of this band can be characterized by a scalar effective mass \( m^* \), then the results derived above are still valid with the proviso that \( m^* \) and the corresponding Fermi velocity are used instead of \( m_e \) and \( v_F \) of free electrons.

The calculations can be extended to solids with more complicated, realistic band structure. We will see that metals, where the Fermi energy lies inside the conduction bands, and semiconductors, where the Fermi energy lies inside the gap between the valence and conduction bands, have essentially different dielectric functions.

### 29.4.1 Dielectric Function of Bloch Electrons

To calculate the dielectric function of the system of Bloch electrons we repeat our earlier derivation of the Lindhard function but now we start with a Bloch state \( \psi_{nk}^{(0)}(r) \) of wave vector \( k \) in the \( n \)th band. The periodically varying external field (29.2.18) couples this state only to those states whose wave vector is \( k + q \) or \( k - q \), though they may be in any band. For this reason, generalizing the trial function given in (29.2.20), the perturbed state is sought in the form

\[
\psi_{nk}(r, t) = \psi_{nk}^{(0)}(r)e^{-i\varepsilon_{nk}t/\hbar} + \sum_{n'} \alpha_{nn'k+q}(t)\psi_{n'k+q}^{(0)}(r)e^{-i\varepsilon_{n'k+q}t/\hbar} + \sum_{n'} \alpha_{nn'k-q}(t)\psi_{n'k-q}^{(0)}(r)e^{-i\varepsilon_{n'k-q}t/\hbar}. \tag{29.4.1}
\]

The coefficient \( \alpha_{nn'k+q}(t) \) can be determined using the formulas of perturbation theory. To lowest order we find

\[
\alpha_{nn'k+q}(t) = \frac{1}{V} \frac{V(q)\langle \psi_{n'k+q}^{(0)} | e^{i\mathbf{q} \cdot \mathbf{r}} | \psi_{nk}^{(0)} \rangle e^{i(\varepsilon_{n'k+q} - \varepsilon_{nk})t/\hbar} e^{-i\omega t} e^{i\delta t}}{-\hbar \omega - \varepsilon_{n'k+q} + \varepsilon_{nk} + i\delta} \tag{29.4.2}
\]

and

\[
\alpha_{nn'k-q}(t) = \frac{1}{V} \frac{V^*(q)\langle \psi_{n'k-q}^{(0)} | e^{-i\mathbf{q} \cdot \mathbf{r}} | \psi_{nk}^{(0)} \rangle e^{i(\varepsilon_{n'k-q} - \varepsilon_{nk})t/\hbar} e^{i\omega t} e^{i\delta t}}{-\hbar \omega - \varepsilon_{n'k-q} + \varepsilon_{nk} + i\delta}. \tag{29.4.3}
\]

Thus, the perturbed wavefunction is...
\( \psi_{n\mathbf{k}}(\mathbf{r}, t) = e^{-i\varepsilon_\mathbf{k} t / \hbar} \psi_{n\mathbf{k}}(\mathbf{r}) \) \hspace{1cm} (29.4.4)

\[ + \frac{1}{V} \sum_{n'} V(q) \sum_{n'k} \frac{V(\mathbf{q})}{\hbar \varepsilon_{n'k} + \varepsilon_{n'k} + i\delta} \psi_{n'k+q}^{(0)}(\mathbf{r}) \psi_{n\mathbf{k}}^{(0)}(\mathbf{r}) e^{-i\varepsilon_{n'k+q} t / \hbar} \]

\[ + \frac{1}{V} \sum_{n'} V^*(\mathbf{q}) \sum_{n'k} \frac{V^*(\mathbf{q})}{\hbar \varepsilon_{n'k} + \varepsilon_{n'k} + i\delta} \psi_{n'k-q}^{(0)}(\mathbf{r}) \psi_{n\mathbf{k}}^{(0)}(\mathbf{r}) e^{-i\varepsilon_{n'k-q} t / \hbar} \].

The essential difference compared to the earlier result for plane waves is that an extra factor appears besides \( V(q) \), the matrix element of \( e^{\pm i\mathbf{q} \cdot \mathbf{r}} \) between \( \psi_{n\mathbf{k}}^{(0)} \) and \( \psi_{n'\mathbf{k} \pm q}^{(0)} \). Using the Bloch form of the electron wavefunction and the lattice periodicity of \( u_{n\mathbf{k}}(\mathbf{r}) \), the matrix element can be written as

\[ \langle \psi_{n'\mathbf{k} + q}^{(0)} | e^{i\mathbf{q} \cdot \mathbf{r}} | \psi_{n\mathbf{k}}^{(0)} \rangle = \frac{1}{v} \int_{v} u_{n'k + q}^*(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}) d\mathbf{r}, \]

where the integration goes over the volume \( v \) of the elementary cell.

The induced density is obtained by summing the absolute square of the wavefunction over all occupied states. Taking its Fourier transform and keeping only the terms proportional to \( V(q) \), the expression for the polarization function is rather similar to (29.2.41) and the dielectric function has a Lindhard-like form,

\[ \epsilon_r(q, \omega) = 1 - 4 \pi \tilde{\varepsilon}_2 2 \sum_{knn'} \frac{f_0(\varepsilon_{nk}) - f_0(\varepsilon_{n'k} + q)}{\hbar \varepsilon_{n'k} + \varepsilon_{nk} + i\delta} \left| \langle \psi_{n'k + q}^{(0)} | e^{i\mathbf{q} \cdot \mathbf{r}} | \psi_{n\mathbf{k}}^{(0)} \rangle \right|^2; \]

however, it contains the absolute square of the matrix element (29.4.5) and besides the summation over \( \mathbf{k} \) one has to sum over the band indices.

In the extended-zone scheme, the states belonging to different zones can be distinguished by an appropriate vector \( \mathbf{G} \) of the reciprocal lattice. Then the dielectric function can be written in the form

\[ \epsilon_r(q, \omega) = 1 - 4 \pi \tilde{\varepsilon}_2 1 \sum_{kG \mathbf{G}' \sigma} \frac{f_0(\varepsilon_{k+G}) - f_0(\varepsilon_{k+q+\mathbf{G}'})}{\hbar \varepsilon_{k+q+\mathbf{G}'} + \varepsilon_{k+G} + i\delta} \times \left| \langle \psi_{k+q+\mathbf{G}'} | e^{i\mathbf{q} \cdot \mathbf{r}} | \psi_{k+G} \rangle \right|^2. \]

\[ \text{29.4.2 Dielectric Constant of Semiconductors} \]

Expression (29.4.6) derived for arbitrary band structure will now be used to calculate the dielectric constant of semiconductors. As has been mentioned already, transitions between the valence and conduction bands play an important role in their optical properties. When their dielectric function is calculated, the states of at least two bands have to be considered. Those terms give a finite contribution in (29.4.6), where the state \( \psi_{n\mathbf{k}}^{(0)} \) is in the valence band and
ψ^{(0)}_{n'k+q} in the conduction band or vice versa. To evaluate the matrix element we consider the double commutator
\[
\left[ [H, e^{iq \cdot r}] -, e^{-iq \cdot r} \right].
\]
(29.4.8)

The lattice-periodic potential in \( H \) commutes with \( e^{iq \cdot r} \), but the operator of kinetic energy does not. Writing explicitly \( -(\hbar^2/2m_e) \nabla^2 \) for the kinetic energy it is readily seen that
\[
\left[ \left[ -\frac{\hbar^2}{2m_e} \nabla^2, e^{iq \cdot r} \right] -, e^{-iq \cdot r} \right] = -\frac{\hbar^2 q^2}{m_e} = -2\varepsilon_q.
\]
(29.4.9)

Alternatively, the diagonal matrix element of the double commutator for state \( \psi^{(0)}_{nk} \) with energy \( \varepsilon_{nk} \) can be calculated by inserting a complete set of intermediate states \( \psi^{(0)}_{n'k'} \). Due to quasimomentum conservation the matrix elements appearing in this expression are nonvanishing only for those intermediate states whose wave vector is equivalent to \( k \pm q \). We get
\[
\langle \psi^{(0)}_{nk} \left| \left[ [H, e^{iq \cdot r}] -, e^{-iq \cdot r} \right] \right| \psi^{(0)}_{nk} \rangle
\]
(29.4.10)
\[
= \sum_{n'} \langle \psi^{(0)}_{nk} | He^{iq \cdot r} | \psi^{(0)}_{n'k'-q} \rangle \langle \psi^{(0)}_{n'k'-q} | e^{-iq \cdot r} | \psi^{(0)}_{nk} \rangle

- \sum_{n'} \langle \psi^{(0)}_{nk} | e^{iq \cdot r} H | \psi^{(0)}_{n'k-q} \rangle \langle \psi^{(0)}_{n'k-q} | e^{-iq \cdot r} | \psi^{(0)}_{nk} \rangle

- \sum_{n'} \langle \psi^{(0)}_{nk} | e^{-iq \cdot r} | \psi^{(0)}_{n'k+q} \rangle \langle \psi^{(0)}_{n'k+q} | He^{iq \cdot r} | \psi^{(0)}_{nk} \rangle

+ \sum_{n'} \langle \psi^{(0)}_{nk} | e^{-iq \cdot r} | \psi^{(0)}_{n'k+q} \rangle \langle \psi^{(0)}_{n'k+q} | e^{iq \cdot r} H | \psi^{(0)}_{nk} \rangle
\]
\[
= \sum_{n'} (\varepsilon_{nk} - \varepsilon_{n'k+q}) \langle \psi^{(0)}_{n'k+q} | e^{iq \cdot r} | \psi^{(0)}_{nk} \rangle^2

+ \sum_{n'} (\varepsilon_{nk} - \varepsilon_{n'k-q}) \langle \psi^{(0)}_{n'k-q} | e^{-iq \cdot r} | \psi^{(0)}_{nk} \rangle^2.
\]
(29.4.11)

Comparison of the two expressions yields
\[
\sum_{n'} (\varepsilon_{n'k+q} - \varepsilon_{nk}) \langle \psi^{(0)}_{n'k+q} | e^{iq \cdot r} | \psi^{(0)}_{nk} \rangle^2

+ \sum_{n'} (\varepsilon_{n'k-q} - \varepsilon_{nk}) \langle \psi^{(0)}_{n'k-q} | e^{-iq \cdot r} | \psi^{(0)}_{nk} \rangle^2 = 2\varepsilon_q.
\]

When the dielectric constant, the value of the dielectric function at \( q \approx 0 \), is considered, the energy difference in the direct transitions between the valence and conduction bands can be approximated by the direct gap,
\[ \varepsilon_{n'k \pm q} - \varepsilon_{nk} \approx \varepsilon_g, \]  
(29.4.12)

when \( k \) is in the valence band and \( k \pm q \) in the conduction band. This is used both in (29.4.11) and in the energy denominator of (29.4.6). The sum over the \( k \) vectors in the valence and conduction bands gives

\[ \varepsilon_r(q, 0) \approx 1 + \frac{4\pi \varepsilon^2}{q^2} \frac{2n_e \varepsilon_q}{\varepsilon_g \varepsilon_g} = 1 + \frac{4\pi n_e e^2}{m^* \varepsilon_g^2} \]  
(29.4.13)

for the dielectric constant where \( n_e \) is the electron density in the valence band. When the density is expressed in terms of the plasma frequency with the help of (16.1.69), we obtain

\[ \varepsilon_r(q, 0) = 1 + \left( \frac{\hbar \omega_p}{\varepsilon_g} \right)^2. \]  
(29.4.14)

The \( 1/q^2 \) singularity characteristic for metals does not appear in semiconductors and the dielectric constant is finite in the limit \( q \to 0 \) owing to the finite gap, the forbidden region around the Fermi energy. As a consequence screening is not complete in semiconductors.

The direct gap is about 4 eV in both Ge and Si, and the plasmon energy is about \( \hbar \omega_p \approx 16 \) eV. This would give \( \varepsilon_r \approx 17 \) for the dielectric constant in good agreement with the experimental values. As mentioned already in Chapter 20, \( \varepsilon_r \approx 12 \) in silicon and \( \varepsilon_r \approx 16 \) in germanium.

### 29.5 Dielectric Function in Special Cases

A very interesting development of the last decades was the discovery of a large class of materials – some of them exist in nature, others could only be synthesized artificially – in which the motion of electrons is confined by the overlap of the wavefunctions of neighboring atoms to only one or two spatial dimensions. This is equivalent to saying that \( \varepsilon_k \) depends in fact on only one or two components of the wave vector. For simplicity we will consider systems where a scalar effective mass can be used, i.e., the dispersion relation has the form

\[ \varepsilon_k = \frac{\hbar^2 k^2}{2m^*} \quad \text{or} \quad \varepsilon_k = \frac{\hbar^2 (k_x^2 + k_y^2)}{2m^*}. \]  
(29.5.1)

The dielectric function will be computed for such systems in the RPA. The response function \( \Pi_0 \) is still defined by (29.2.41), but its value, which can be given in closed form for both one- and two-dimensional systems,\(^7\) depends strongly on the dimensionality of the phase space. Finally we will discuss the case when the Fermi surface has a nesting property. Even though the motion of the electrons is not restricted to one or two directions, a singularity characteristic of one-dimensional systems appears in the dielectric function.

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\(^7\) The results will be given by replacing the effective mass with the electron mass.
29.5.1 Dielectric Function of the Two-Dimensional Electron Gas

The dielectric function of the two-dimensional electron gas will be written in analogy to (29.2.54) in the form

$$\epsilon_r(q, \omega) = 1 + \frac{4\pi\tilde{e}^2}{q^2} \rho_{2d}(\varepsilon_F) F_{2d}(q, \omega),$$  \hspace{1cm} (29.5.2)

where $\rho_{2d}(\varepsilon_F) = \frac{m_e}{\pi \hbar^2}$ is the density of states of the two-dimensional electron gas. In a strictly two-dimensional system, solution of the Poisson equation gives $U(q) = \frac{2\pi e^2}{q}$ for the Fourier transform of the Coulomb potential. Nonetheless, we use the choice given above since we are considering a truly three-dimensional system, in which, however, the electrons can propagate with high probability in two directions only. We first consider the region of momenta $q < 2k_F$ where $\hbar v_F q > \varepsilon_q$. One has to distinguish again three frequency ranges. Separating $F_{2d}(q, \omega)$ into real and imaginary parts in the form $F'_{2d} + iF''_{2d}$, in the low-frequency range $0 \leq \hbar \omega < \hbar v_F q - \varepsilon_q$ we have

$$F'_{2d}(q, \omega) = 1$$  \hspace{1cm} (29.5.3)

and

$$F''_{2d}(q, \omega) = \frac{[(\hbar q v_F)^2 - (\varepsilon_q - \hbar \omega)^2]^{1/2}}{2\varepsilon_q} - \frac{[(\hbar q v_F)^2 - (\varepsilon_q + \hbar \omega)^2]^{1/2}}{2\varepsilon_q}.$$  \hspace{1cm} (29.5.4)

For intermediate frequencies satisfying $\hbar v_F q - \varepsilon_q \leq \hbar \omega \leq \hbar v_F q + \varepsilon_q$ we find

$$F'_{2d}(q, \omega) = 1 - \frac{[(\varepsilon_q + \hbar \omega)^2 - (\hbar q v_F)^2]^{1/2}}{2\varepsilon_q}$$  \hspace{1cm} (29.5.5)

and

$$F''_{2d}(q, \omega) = \frac{[(\hbar q v_F)^2 - (\varepsilon_q - \hbar \omega)^2]^{1/2}}{2\varepsilon_q}.$$  \hspace{1cm} (29.5.6)

Finally, at high frequencies where $\hbar v_F q + \varepsilon_q \leq \hbar \omega$ we have

$$F'_{2d}(q, \omega) = 1 - \frac{[(\varepsilon_q + \hbar \omega)^2 - (\hbar q v_F)^2]^{1/2}}{2\varepsilon_q} + \frac{[(\hbar \omega - \varepsilon_q)^2 - (\hbar q v_F)^2]^{1/2}}{2\varepsilon_q}$$  \hspace{1cm} (29.5.7)

and

$$F''_{2d}(q, \omega) = 0.$$  \hspace{1cm} (29.5.8)

Similar expressions are obtained for $q > 2k_F$ where $\varepsilon_q > \hbar q v_F$. At low frequencies, in the range $0 \leq \hbar \omega < \varepsilon_q - \hbar v_F q$,

$$F'_{2d}(q, \omega) = 1 - \frac{[(\varepsilon_q + \hbar \omega)^2 - (\hbar q v_F)^2]^{1/2}}{2\varepsilon_q} - \frac{[(\varepsilon_q - \hbar \omega)^2 - (\hbar q v_F)^2]^{1/2}}{2\varepsilon_q}$$  \hspace{1cm} (29.5.9)
and
\[ F'_{2d}(q, \omega) = 0, \quad (29.5.10) \]
in the intermediate frequency range \( \varepsilon_q - \hbar v_F q \leq \hbar \omega \leq \varepsilon_q + \hbar v_F q \) we find
\[ F''_{2d}(q, \omega) = 1 - \left[ \frac{(\varepsilon_q + \hbar \omega)^2 - (\hbar q v_F)^2}{2 \varepsilon_q} \right]^{1/2}, \quad (29.5.11) \]
and
\[ F''_{2d}(q, \omega) = \frac{[(\hbar q v_F)^2 - (\varepsilon_q - \hbar \omega)^2]^{1/2}}{2 \varepsilon_q}, \quad (29.5.12) \]
while in the high-frequency range \( \varepsilon_q + \hbar v_F q \leq \hbar \omega \)
\[ F'_{2d}(q, \omega) = 1 - \left[ \frac{(\varepsilon_q + \hbar \omega)^2 - (\hbar q v_F)^2}{2 \varepsilon_q} \right]^{1/2} + \left[ \frac{(\varepsilon_q - \hbar \omega)^2 - (\hbar q v_F)^2}{2 \varepsilon_q} \right]^{1/2}, \quad (29.5.13) \]
and
\[ F''_{2d}(q, \omega) = 0. \quad (29.5.14) \]
In the static limit, the function \( F(q) \) takes the form
\[ F_{2d}(q) = \begin{cases} 1 & \text{for } q < 2k_F, \\ 1 - \sqrt{1 - (2k_F/q)^2} & \text{for } q > 2k_F. \end{cases} \quad (29.5.15) \]

29.5.2 Dielectric Function of the One-Dimensional Electron Gas

The polarization function of a one-dimensional electron gas is again given by (29.2.31). If \( q < 2k_F \), two regions, \( k_F - q \leq k \leq k_F \) and \(-k_F - q \leq k \leq -k_F \) (see Fig. 29.9), give finite contribution in the integral. Otherwise either both Fermi distribution functions take unit value or both vanish.

\[ \text{Fig. 29.9. The “Fermi spheres” belonging to the wave numbers } k \text{ and } k + q. \text{ Only the regions covered once give finite contributions to the Lindhard function.} \]
We get

\[
\Re \Pi_0(q, \omega) = \frac{1}{\pi} \int_{k_F - q}^{k_F} \frac{dk}{\hbar \omega - \hbar^2 k/m_e - \varepsilon_q} - \frac{1}{\pi} \int_{-k_F}^{-k_F - q} \frac{dk}{\hbar \omega - \hbar^2 k/m_e - \varepsilon_q} - \frac{1}{\pi} \int_{k_F}^{k_F - q} \frac{dk}{\hbar \omega - \hbar^2 k/m_e - \varepsilon_q}
\]

\[
= -\frac{1}{\pi} \frac{m_e}{\hbar^2 q} \ln \left| \frac{\hbar v_F q + \varepsilon_q - \hbar \omega}{\hbar v_F q - \varepsilon_q + \hbar \omega} \right| - \ln \left| \frac{\hbar v_F q - \varepsilon_q + \hbar \omega}{\hbar v_F q + \varepsilon_q + \hbar \omega} \right|
\]

\[
= -\frac{1}{\pi} \frac{m_e}{\hbar^2 q} \ln \left| \frac{(\hbar v_F q + \varepsilon_q)^2 - (\hbar \omega)^2}{(\hbar v_F q - \varepsilon_q)^2 - (\hbar \omega)^2} \right|
\]  
\[\text{(29.5.16)}\]

for the real part. If \( q > 2k_F \), the integration goes over two full “Fermi spheres”. We then have

\[
\Re \Pi_0(q, \omega) = \frac{1}{\pi} \int_{-k_F}^{k_F} \frac{dk}{\hbar \omega - \hbar^2 k/m_e - \varepsilon_q} - \frac{1}{\pi} \int_{-k_F}^{-k_F - q} \frac{dk}{\hbar \omega - \hbar^2 k/m_e - \varepsilon_q}
\]

\[
= -\frac{1}{\pi} \frac{m_e}{\hbar^2 q} \ln \left| \frac{\hbar v_F q + \varepsilon_q - \hbar \omega}{-\hbar v_F q + \varepsilon_q - \hbar \omega} \right| - \ln \left| \frac{\hbar v_F q - \varepsilon_q - \hbar \omega}{-\hbar v_F q - \varepsilon_q - \hbar \omega} \right|
\]

\[
= -\frac{1}{\pi} \frac{m_e}{\hbar^2 q} \ln \left| \frac{(\hbar v_F q + \varepsilon_q)^2 - (\hbar \omega)^2}{(\hbar v_F q - \varepsilon_q)^2 - (\hbar \omega)^2} \right|
\]  
\[\text{(29.5.17)}\]

The imaginary part, too, can be easily calculated yielding

\[
\Im \Pi_0(q, \omega) = \begin{cases} 
0 & \text{for } 0 \leq \hbar \omega < \hbar v_F q - \varepsilon_q, \\
-\frac{m_e}{\hbar^2 k_F} & \text{for } \hbar v_F q - \varepsilon_q \leq \hbar \omega \leq \hbar v_F q + \varepsilon_q, \\
0 & \text{for } \hbar v_F q + \varepsilon_q \leq \hbar \omega.
\end{cases}
\]  
\[\text{(29.5.18)}\]

We can write again the response function in the form

\[
\Pi_0(q, \omega) = -\rho_{1d}(\varepsilon_F) F_{1d}(q, \omega),
\]  
\[\text{(29.5.19)}\]

where

\[
\rho_{1d}(\varepsilon_F) = \frac{2m_e}{\pi \hbar^2 k_F^2}
\]  
\[\text{(29.5.20)}\]

is the density of states of the one-dimensional electron gas at the Fermi energy and

\[
\Re F_{1d}(q, \omega) = \frac{k_F}{2q} \ln \left| \frac{(\hbar v_F q + \varepsilon_q)^2 - (\hbar \omega)^2}{(\hbar v_F q - \varepsilon_q)^2 - (\hbar \omega)^2} \right|
\]  
\[\text{(29.5.21)}\]

In the static limit, this quantity reduces to

\[
F_{1d}(q) = \frac{k_F}{q} \ln \left| \frac{2k_F + q}{2k_F - q} \right|
\]  
\[\text{(29.5.22)}\]

The results obtained for \( F(x) \) with \( x = q/2k_F \) for the one-, two-, and three-dimensional cases are plotted in Fig. 29.10.
29.5 Dielectric Function in Special Cases

The function $F(x)$ displays stronger and stronger singularities at $x = 1$ ($q = 2k_F$) as the dimensionality decreases. It is continuous in the two- and three-dimensional cases and only its derivative is singular at $x = 1$. The function $F$ itself is singular at this point in the one-dimensional case. The reason for this singular behavior is easy to find when we look at (29.2.31). As described by the Fermi distribution functions, the hole with wave vector $k$ has to be created inside the Fermi sphere and the electron with $k + q$ outside or the role of the electron and the hole can be interchanged. When two Fermi spheres shifted by a vector $-q$ are drawn as in Fig. 29.11, the integrand vanishes outside the shaded region. The region inside the Fermi sphere around the origin appears with weight $+1$ in the integrand, whereas the region inside the Fermi sphere around the tip of the vector $-q$ with weight $-1$.

Taking $\omega = 0$ at a fixed value of $q$ the energy denominator in the Lindhard function vanishes at those $k$ vectors for which $\varepsilon_{k+q} = \varepsilon_k$. This condition is satisfied in a tiny portion of the region of integration in the three-dimensional case, along the intersection of the two displaced Fermi spheres, where both the electron and the hole are on the Fermi surface. The integrand is large in the neighborhood of this circle, but only in a tiny portion of the phase space.
The response function is thus a continuous function and only its derivative shows a weak, logarithmic singularity at \( q = 2k_F \).

In two-dimensional systems the energy denominator vanishes at two points, at the intersection of the two Fermi circles. The integral itself remains finite; however, the derivative of the response function displays a stronger singularity, it is discontinuous at \( q = 2k_F \). The integrand is singular at two points of the phase space in the one-dimensional case as well, but this singularity is not compensated by the smallness of the corresponding phase space. The response function itself is singular at \( q = 2k_F \).

**29.5.3 Materials with Nested Fermi Surface**

We may ask what happens when the electron system is three dimensional, but the shape of the Fermi surface deviates significantly from the sphere. We consider as an example a crystal with orthorhombic structure where the energy of electron states in the tight-binding approximation is given by

\[
\varepsilon_k = \varepsilon_0 + \varepsilon_1 \cos k_x a + \varepsilon_2 \cos k_y b + \varepsilon_3 \cos k_z c. 
\]  

(29.5.23)

It may occur that in two of the crystallographic directions (say in the \( y \)- and \( z \)-directions) the overlap of the wavefunctions of neighboring atoms is much weaker than in the third direction, \(|\varepsilon_1| \gg |\varepsilon_2|, |\varepsilon_3|\), and also that \(|\varepsilon_2| \gg |\varepsilon_3|\). In such systems there is a preferred direction of propagation. Electrons move in one direction with much higher probability than in the other directions. The system can be considered electronically quasi-one-dimensional. If the term proportional to \( \varepsilon_1 \) is approximated by a linear spectrum near the Fermi energy and the smallest term proportional to \( \varepsilon_3 \) is neglected, the dispersion relation becomes

\[
\varepsilon_k = \varepsilon_0 + \hbar v_F (\pm k_x - k_F) + \varepsilon_2 \cos k_y b, 
\]  

(29.5.24)

where the \(+\) sign has to be chosen for \( k_x \) close to \( k_F \) and the \(-\) sign when \( k_x \) is close to \(-k_F\). Figure 29.12 shows the Fermi surface corresponding to this spectrum. It is seen that the Fermi surface consists of two parts, which appear as two sheets.

It is easy to verify that if the left sheet of the Fermi surface is shifted by the vector

\[
\mathbf{q}_0 = (2k_F, \pi/b),
\]  

(29.5.25)

it will exactly coincide with the right sheet, provided that, if necessary, the wave vectors are reduced to the first Brillouin zone. Evaluating the response function at this \( \mathbf{q}_0 \), the energy denominator vanishes for all \( \mathbf{k} \) vectors lying on the left sheet of the Fermi surface and the response function is singular at \( \mathbf{q} = \mathbf{q}_0 \). The same logarithmic singularity appears as in one-dimensional systems.

Such a divergence may appear not only in quasi-one-dimensional systems. As has been seen already in Fig. 18.23, the “Fermi sphere” is distorted to a
Fig. 29.12. Fermi surface of a quasi-one-dimensional system with the nesting vector square in the tight-binding approximation for a two-dimensional square lattice if the band is half filled. Opposite edges of the Fermi surface are separated by one of the vectors \( q_0 = (\pm \pi/a, \pm \pi/a) \). If the response function is calculated at this \( q_0 \), the energy denominator vanishes for every vector \( k \) of the edge of the Fermi surface under consideration and therefore the response function exhibits similar logarithmic singularities.

These examples show that the divergence is the consequence of the special shape of the Fermi surface, namely, when the Fermi surface is displaced by an appropriately chosen wave vector \( q_0 \), an extended region of the Fermi surface has to coincide (nest) with another portion of the Fermi surface. Such Fermi surfaces are said to have the property of *nesting*. Figure 29.13 shows two further examples of nested Fermi surfaces.

Fig. 29.13. Nested Fermi surfaces with the nesting vector

When the dielectric response of such systems is calculated at the nesting vector \( q_0 \), the energy denominator vanishes along the whole nesting region, and therefore the response function has the same kind of logarithmic singularity as the one-dimensional model at \( 2k_F \). This singularity may lead to the appearance of a new state, a static charge-density-wave or spin-density-wave state. This problem will be treated in Chapter 33.
29.6 Response to Electromagnetic Field

In the foregoing the response of the electron system to an external charge or scalar potential was studied. This could have been described equivalently as the response to a longitudinal vector potential, since according to (29.1.15) both the electric field and the electric displacement are parallel to the wave vector \( \mathbf{q} \). The dielectric function and the conductivity determined in this way are thus responses to longitudinal perturbations. A different situation is encountered when the optical properties are considered, since in a radiating electromagnetic field the vectors \( \mathbf{E} \) and \( \mathbf{H} \) are perpendicular to the direction of propagation. The ratio of the perpendicular components of \( \mathbf{D} \) and \( \mathbf{E} \) gives the transverse dielectric function \( \epsilon_{\perp} = \epsilon_{\perp}/\epsilon_0 \), where \( \epsilon_{\perp} \) was defined in (29.1.6) and (29.1.8). This quantity is not necessarily the same as the longitudinal dielectric function even if the medium is isotropic. More importantly, the transverse electromagnetic field couples to the current and therefore the response of the electron system to such perturbations can be described by the current–current response function. We will derive the Kubo formula that expresses the conductivity in terms of the retarded current–current correlation function and will specify it for the optical and DC conductivities.

29.6.1 Interaction with the Electromagnetic Field

The interaction between the electron system and an electromagnetic field can be derived from the Hamiltonian of the interacting electron system in the presence of an electromagnetic field. If the field is described by a scalar potential \( \varphi(\mathbf{r}) \) and a vector potential \( \mathbf{A}(\mathbf{r}) \), we have

\[
\mathcal{H} = \frac{1}{2m_e} \sum_{i=1}^{N_e} \left[ \mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i) \right]^2 - e \sum_{i=1}^{N_e} \varphi(\mathbf{r}_i) + \frac{1}{2} \sum_{i,j=1}^{N_e} \frac{\mathbf{E}_i^2}{|\mathbf{r}_i - \mathbf{r}_j|} ,
\]

(29.6.1)

where the kinetic energy is given in terms of the kinetic momentum \( \mathbf{p} + e\mathbf{A} \) instead of the canonical momentum \( \mathbf{p} \). Subtracting from this expression the terms not related to the electromagnetic field, the remaining terms collected into

\[
\mathcal{H}_1 = \sum_i \left\{ \frac{e}{2m_e} [\mathbf{A}(\mathbf{r}_i) \cdot \mathbf{p}_i + \mathbf{p}_i \cdot \mathbf{A}(\mathbf{r}_i)] + \frac{e^2}{2m_e} A^2(\mathbf{r}_i) - e\varphi(\mathbf{r}_i) \right\}
\]

(29.6.2)

\[
= \sum_i \left\{ \frac{e\hbar}{2im_e} [\mathbf{A}(\mathbf{r}_i) \cdot \nabla_i + \nabla_i \cdot \mathbf{A}(\mathbf{r}_i)] + \frac{e^2}{2m_e} A^2(\mathbf{r}_i) - e\varphi(\mathbf{r}_i) \right\}
\]

describe the interaction. It is convenient to work in Coulomb (transverse) gauge, where \( \text{div} \mathbf{A} = 0 \), i.e., the vector potential is perpendicular to the propagation vector \( \mathbf{q} \) and the scalar potential vanishes. When only the terms
linear in the vector potential are kept, the interaction Hamiltonian can be written in the simple form
\[ \mathcal{H}_1 = -\int \hat{j}(r) \cdot A(r, t) \, dr, \quad (29.6.3) \]
where \( \hat{j}(r) \) is the operator of the current density. To substantiate this statement we recall that the quantum mechanical expression for the operator of the particle-current density is
\[ \hat{j}_n(r) = \frac{1}{2m_e} \sum_i [p_i \delta(r - r_i) + \delta(r - r_i) p_i] \quad (29.6.4) \]
and the electric-current operator is
\[ \hat{j}(r) = -e \hat{j}_n(r) = -\frac{e}{2m_e} \sum_i [p_i \delta(r - r_i) + \delta(r - r_i) p_i]. \quad (29.6.5) \]
This shows that the perturbing vector potential couples indeed to the current. Expressing the vector potential and the current in terms of their Fourier components, one readily finds
\[ \mathcal{H}_1 = -\frac{1}{V} \sum_q \hat{j}(-q) \cdot A(q, t), \quad (29.6.6) \]
where
\[ \hat{j}(q) = -\frac{e}{2m_e} \frac{\hbar}{i} \sum_i [\nabla_i e^{-i q \cdot r_i} + e^{-i q \cdot r_i} \nabla_i], \quad (29.6.7) \]
or in second-quantized form
\[ \hat{j}(q) = -\frac{e \hbar}{m_e} \sum_{k \sigma} (k + \frac{1}{2} q) c_{k\sigma}^\dagger c_{k+q\sigma} = -\frac{e \hbar}{m_e} \sum_{k \sigma} k c_{k-q/2 \sigma}^\dagger c_{k+q/2 \sigma}. \quad (29.6.8) \]
Before going on we have to recognize that the expression given above for the current density is valid in the absence of electromagnetic field. In its presence it has to be modified to make it gauge invariant. The correct expression should contain the kinetic momentum
\[ \hat{j}(r) = -\frac{e}{2m_e} \sum_i \left\{ [p_i + eA(r_i)] \delta(r - r_i) + \delta(r - r_i) [p_i + eA(r_i)] \right\} \]
\[ = -\frac{e}{2m_e} \sum_i [p_i \delta(r - r_i) + \delta(r - r_i) p_i] - \frac{e^2}{m_e} \sum_i A(r_i) \delta(r - r_i). \quad (29.6.9) \]
The total current operator can be decomposed naturally into two terms:
\[ \hat{j} = \hat{j}_p + \hat{j}_d, \quad (29.6.10) \]
where
\[ \hat{j}_p(r) = -\frac{e}{2m_e} \sum_i \left[ p_i \delta(r - r_i) + \delta(r - r_i)p_i \right] \] (29.6.11)
is the so-called paramagnetic current; it is the current component that appears in the interaction with the electromagnetic field to lowest order in the field, while the second term,
\[ \hat{j}_d(r) = -\frac{e^2}{m_e} \sum_i A(r_i) \delta(r - r_i) \] (29.6.12)
is the diamagnetic current. This term can be written in terms of the electron density as
\[ \hat{j}_d(r) = -\frac{e^2}{m_e} A(r)n(r) \] (29.6.13)

29.6.2 Current–Current Correlations and the Kubo Formula

The total current density is the expectation value of the current operator. In what follows the notation \( \hat{j} \) will be used for the total current density and \( \hat{j} \) for the operator of the paramagnetic current. We then have
\[ j(r, t) = \langle \hat{j}(r, t) \rangle - \frac{n_e e^2}{m_e} A(r, t) \] (29.6.14)
if the electric field is time dependent, and the particle density has been replaced with its unperturbed mean value. Assuming a periodically varying space and time dependence for the vector potential with a fixed frequency and wave vector,
\[ A(r, t) = A(q, t)e^{iq \cdot r} = A(q)e^{i(q \cdot r - \omega t)} \] (29.6.15)
the current varies with the same periodicity, and the spatial Fourier transform of the current density is
\[ j(q, t) = \langle \hat{j}(q, t) \rangle - \frac{n_e e^2}{m_e} A(q) \] (29.6.16)
The current at a given frequency is the Fourier transform of this quantity, that is
\[ j(q, \omega) = \langle \hat{j}(q, \omega) \rangle - \frac{n_e e^2}{m_e} A(q, \omega) \] (29.6.17)
For weak external perturbations the current is proportional to the internal electric field. In the most general case
\[ j_\alpha(r, t) = \sum_\beta \int dt' \int_{-\infty}^{t} dt' \sigma_{\alpha\beta}(r, r', t - t') E_\beta(r', t') \] (29.6.18)
where $\sigma_{\alpha\beta}$ is the conductivity tensor. In a homogeneous system the relationship is algebraic between the Fourier components:

$$j(q, \omega) = \sigma(q, \omega)E(q, \omega).$$  \hspace{1cm} (29.6.19)

Note that the relationship between current and electric field is causal; hence, the Kramers–Kronig relations are satisfied by the real and imaginary parts of the conductivity:

$$\text{Re} \sigma(q, \omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \frac{\text{Im} \sigma(q, \omega')}{\omega' - \omega},$$  \hspace{1cm} (29.6.20)

$$\text{Im} \sigma(q, \omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \frac{\text{Re} \sigma(q, \omega')}{\omega' - \omega} = \frac{2\omega}{\pi} P \int_{0}^{\infty} d\omega' \frac{\text{Re} \sigma(q, \omega')}{\omega'^2 - \omega^2}.$$  \hspace{1cm} (29.6.21)

To derive the conductivity, the paramagnetic current has to be calculated as a linear response to the perturbing electromagnetic field. Since the mean value of the paramagnetic current has to be calculated and the vector potential couples to the same paramagnetic component of the current, the response function that connects the current to the vector potential in the expression

$$\langle \hat{j}_\alpha(r, t) \rangle = -\int_{-\infty}^{t} dt' \int dr' P_{\alpha\beta}(r, r', t - t') A_\beta(r', t')$$  \hspace{1cm} (29.6.22)

is the current–current response function:

$$P_{\alpha\beta}(r, r', t - t') = -\frac{i}{\hbar} \theta(t - t') \langle \hat{j}_\alpha(r, t), \hat{j}_\beta(r', t') \rangle.$$  \hspace{1cm} (29.6.23)

In a homogeneous system where the response depends only on $r - r'$, the Fourier transform of the paramagnetic current density is

$$\langle \hat{j}_\alpha(q, \omega) \rangle = -P_{\alpha\beta}(q, \omega) A_\beta(q, \omega),$$  \hspace{1cm} (29.6.24)

where

$$P_{\alpha\beta}(q, \omega) = -\frac{i}{\hbar V} \int_{-\infty}^{\infty} dt e^{i\omega t} \theta(t - t') \langle \hat{j}_\alpha(q, t), \hat{j}_\beta(-q, t') \rangle.$$  \hspace{1cm} (29.6.25)

The retarded response function has to be analytic in the upper complex $\omega$ half-plane. This is achieved by inserting a factor $\exp(-\delta t)$ with a positive
infinitesimal $\delta$ in the last integrand. This factor corresponds to switching on the perturbation adiabatically. We thus have

$$P_{\alpha\beta}(q, \omega) = -\frac{i}{\hbar} \frac{1}{V} \int_0^\infty dt e^{i\omega t - \delta t} \left\langle \left[ \hat{j}_\alpha(q, t), \hat{j}_\beta(-q, 0) \right] \right\rangle. \quad (29.6.25)$$

When the average is calculated at finite temperatures in terms of the matrix elements between the complete set of eigenstates of the unperturbed Hamiltonian, we find

$$P_{\alpha\beta}(q, \omega) = \frac{1}{V} \sum_{mn} \left( \frac{e^{-\beta E_n}}{Z} - \frac{e^{-\beta E_m}}{Z} \right) \frac{\langle \Psi_n | \hat{j}_\alpha(q) | \Psi_m \rangle \langle \Psi_m | \hat{j}_\beta(-q) | \Psi_n \rangle}{\hbar \omega - E_m + E_n + i\delta}. \quad (29.6.26)$$

The current–current correlation function appears in response to the vector potential, while the conductivity is defined through the response to the electric field. We make use of the relationship

$$E(r, t) = -\frac{\partial A(r, t)}{\partial t} \quad (29.6.27)$$

valid in that gauge where the scalar potential vanishes. For fields varying with frequency $\omega$, this leads to

$$E(r, \omega) = i\omega A(r, \omega). \quad (29.6.28)$$

Substituting this into (29.6.23) and adding the paramagnetic and diamagnetic contributions we have

$$\sigma_{\alpha\beta}(q, \omega) = \frac{i}{\omega} \left[ P_{\alpha\beta}(q, \omega) + \frac{n_e e^2}{m_e} \delta_{\alpha\beta} \right]. \quad (29.6.29)$$

With the explicit form of the current–current response function $P_{\alpha\beta}$ we find the relationship

$$\sigma_{\alpha\beta}(q, \omega) = \frac{1}{\hbar \omega} \frac{1}{V} \int_0^\infty dt e^{i(\omega + i\delta)t} \left\langle \left[ \hat{j}_\alpha(q, t), \hat{j}_\beta(-q, 0) \right] \right\rangle + \frac{i n_e e^2}{m_e \omega} \delta_{\alpha\beta}. \quad (29.6.30)$$

known as the *Kubo formula*.\(^8\) In real-space representation

\(^8\) R. Kubo, 1957. The name Kubo formula refers more generally to the formula that expresses the generalized susceptibility as a retarded correlation function. This is discussed in more detail in Appendix J. The expression for transport coefficients is often referred to as Green–Kubo formula (M. S. Green, 1952, 1954), while the expression for the conductivity is sometimes referred to as Kubo–Nakano formula (H. Nakano, 1956).
\[
\sigma_{\alpha\beta}(\mathbf{r}, \mathbf{r}', \omega) = \frac{1}{\hbar \omega} \int_0^\infty dt \, e^{i(\omega + i\delta)t} \left\langle \left[ \hat{j}_\alpha(\mathbf{r}, t), \hat{j}_\beta(\mathbf{r}', 0) \right] \rightangle + \frac{i n_e e^2}{m_e \omega} \delta_{\alpha\beta} \delta(\mathbf{r} - \mathbf{r}').
\]

(29.6.31)

If the thermal average is written in terms of the matrix elements between a complete set of states \(|\Psi_n\rangle\) of energy \(E_n\), as in (29.6.26), we find

\[
\sigma_{\alpha\beta}(\mathbf{q}, \omega) = \frac{i}{\omega} \sum_{mn} \left( \frac{e^{-\beta E_n}}{Z} - \frac{e^{-\beta E_m}}{Z} \right) \frac{\langle \Psi_n | \hat{j}_\alpha(\mathbf{q}) | \Psi_m \rangle \langle \Psi_m | \hat{j}_\beta(-\mathbf{q}) | \Psi_n \rangle}{\hbar \omega - E_m + E_n + i\delta} + \frac{i n_e e^2}{m_e \omega} \delta_{\alpha\beta}.
\]

(29.6.32)

The real part of the frequency-dependent conductivity can then be written as

\[
\text{Re} \, \sigma_{\alpha\beta}(\mathbf{q}, \omega) = \frac{\pi}{\omega} \sum_{mn} \left( \frac{e^{-\beta E_n}}{Z} - \frac{e^{-\beta E_m}}{Z} \right) \frac{\langle \Psi_n | \hat{j}_\alpha(\mathbf{q}) | \Psi_m \rangle \langle \Psi_m | \hat{j}_\beta(-\mathbf{q}) | \Psi_n \rangle}{\hbar \omega - E_m + E_n + i\delta} \times \langle \Psi_m | \hat{j}_\beta(-\mathbf{q}) | \Psi_n \rangle \delta(\hbar \omega - E_m + E_n).
\]

(29.6.33)

Alternatively this expression could have been derived by making use of the fact that the real part of the conductivity is proportional to the imaginary part of the current–current response function

\[
\text{Re} \, \sigma_{\alpha\beta}(\mathbf{q}, \omega) = -\frac{1}{\omega} \text{Im} \, P_{\alpha\beta}(\mathbf{q}, \omega),
\]

(29.6.34)

which in turn can be expressed in terms of the current–current correlation function using the fluctuation–dissipation theorem outlined in Appendix J:

\[
\frac{1}{V} \int_{-\infty}^{\infty} dt \, e^{i\omega t} \langle \hat{j}_\alpha(\mathbf{q}, t) \hat{j}_\beta(-\mathbf{q}, 0) \rangle = -\frac{2\hbar}{1 - e^{-\beta \hbar \omega}} \text{Im} \, P_{\alpha\beta}(\mathbf{q}, \omega).
\]

(29.6.35)

We then find that

\[
\text{Re} \, \sigma_{\alpha\beta}(\mathbf{q}, \omega) = \frac{1}{2\hbar \omega} (1 - e^{-\beta \hbar \omega}) \frac{1}{V} \int_{-\infty}^{\infty} dt \, e^{i\omega t} \langle \hat{j}_\alpha(\mathbf{q}, t) \hat{j}_\beta(-\mathbf{q}, 0) \rangle.
\]

(29.6.36)

If the thermal average is written in terms of the matrix elements between a complete set of states with the appropriate weight factor, the time integral can be performed using
\[ \int_{-\infty}^{\infty} e^{i\omega t} \, dt = 2\pi \delta(\omega) \] \hspace{1cm} (29.6.37)

and we find precisely (29.6.33).

### 29.6.3 Transverse and Longitudinal Response

In the derivation of the Kubo formula the response to an external electric field was considered. When the conductivity is calculated, we have to take into account that the current is the response to the internal field \( E \). We show that this leads to the expression

\[ \sigma_{\alpha\beta}(q, \omega) = \frac{i}{\omega} \left[ \tilde{P}_{\alpha\beta}(q, \omega) + \frac{n_e e^2}{m_e} \delta_{\alpha\beta} \right] \] \hspace{1cm} (29.6.38)

for the conductivity tensor instead of (29.6.29), where \( \tilde{P}_{\alpha\beta}(q, \omega) \) is the irreducible part of \( P_{\alpha\beta}(q, \omega) \).

First, we show that this makes no difference for the transverse response since transverse fields are not screened. This can be best seen when the current–current response function is visualized by diagrams. These diagrams have the same form as the diagrams for the density–density response function; their analytic expression is, however, different. The current vertex (its analytic form can be inferred from the second-quantized expression for the current operator) appears at the two end points, where the electron–hole pair is created and annihilated. Analogous to the density–density response function, one can distinguish irreducible and reducible processes in the current–current response function, too. The reducible diagrams can be separated into two unconnected parts by cutting a single appropriately chosen interaction line. The diagrams for the full response function form again a geometric progression, in which irreducible polarization bubbles are coupled to each other by interaction lines, similar to the diagrammatic representation of the density–density correlation function, except that the first and last bubbles have a current vertex; they represent the irreducible part of the current–density and the density–current response functions

\[ S_{\alpha}(q, \omega) = -\frac{i}{\hbar} \frac{1}{V} \int_{0}^{\infty} dt e^{i\omega t - \delta t} \left\langle \left[ \hat{j}_{\alpha}(q, t), n(-q, 0) \right] \right\rangle \] \hspace{1cm} (29.6.39)

and

\[ \overline{S}_{\alpha}(q, \omega) = -\frac{i}{\hbar} \frac{1}{V} \int_{0}^{\infty} dt e^{i\omega t - \delta t} \left\langle \left[ n(q, t), \hat{j}_{\alpha}(-q, 0) \right] \right\rangle . \] \hspace{1cm} (29.6.40)

Denoting their irreducible parts by \( \tilde{S}_{\alpha}(q, \omega) \) and \( \bar{S}_{\alpha}(q, \omega) \), respectively, and the irreducible part of the current–current response function by \( P_{\alpha\beta} \), we have
\[ P_{\alpha\beta}(q, \omega) = \tilde{P}_{\alpha\beta}(q, \omega) + \tilde{S}_\alpha(q, \omega) \frac{4\pi e^2 / q^2}{1 - (4\pi e^2 / q^2) \tilde{P}}(q, \omega). \]  

(29.6.41)

The current–density response function being a vector, its components perpendicular to \( q \) vanish by symmetry in an isotropic system,

\[ S_\perp(q, \omega) = \tilde{S}_\perp(q, \omega) = 0, \]  

(29.6.42)

and therefore

\[ P_\perp(q, \omega) = \tilde{P}_\perp(q, \omega). \]  

(29.6.43)

This shows that there are no polarization corrections to the transverse response; the transverse vector potential and transverse fields are not screened. Thus

\[ \sigma_\perp(q, \omega) = i \omega \left[ P_\perp(q, \omega) + \frac{n_ie^2}{m_e} \right] = i \omega \left[ \tilde{P}_\perp(q, \omega) + \frac{n_ie^2}{m_e} \right]. \]  

(29.6.44)

The situation is different for the longitudinal response. To see that we rewrite the interaction of the electron system with an external potential,

\[ \mathcal{H}_1 = \int n(r)V_{\text{ext}}(r, t) \, dr = -e \int n(r)\varphi_{\text{ext}}(r, t) \, dr = -e V \sum_q n(-q)\varphi_{\text{ext}}(q, t), \]  

(29.6.45)

in terms of a longitudinal vector potential by making use of the gauge invariance of electrodynamics. The same longitudinal electric field is obtained from the longitudinal vector potential defined by

\[ -\nabla \varphi_{\text{ext}}(r, t) = -\frac{\partial A_{\text{ext}}(r, t)}{\partial t}. \]  

(29.6.46)

Assuming that the longitudinal field varies periodically in space and time we have the relationship

\[ q\varphi_{\text{ext}}(q, \omega) = -\omega A_{\text{ext}}(q, \omega) \]  

(29.6.47)

between the Fourier components. On the other hand, the number density and the particle-current density have to satisfy the continuity equation

\[ \frac{\partial n(r, t)}{\partial t} + \text{div} \, \hat{j}_n(r, t) = 0 \]  

(29.6.48)

that follows from the particle-number (charge) conservation. This implies

\[ \omega n(q, t) = q \cdot \hat{j}_n(q, t). \]  

(29.6.49)

Substituting these relations into (29.6.45) we see that in the longitudinal case as well
\[
\mathcal{H}_1 = \frac{e}{V} \sum_q \hat{j}_n(-q) \cdot A(q,t) = -\frac{1}{V} \sum_q \hat{j}(-q) \cdot A(q,t) = -\int \hat{j}(r) A(r,t) \, dr.
\] (29.6.50)

If the vector potential and the current are parallel to \( q \), the relationship
\[
\langle \hat{j}(q, \omega) \rangle = -P_\parallel(q, \omega) A_{\text{ext}}(q, \omega)
\] (29.6.51)
defines the longitudinal current–current response function, and the total current is given by
\[
j(q, \omega) = -\left[ P_\parallel(q, \omega) + \frac{n_e e^2}{m_e} \right] A_{\text{ext}}(q, \omega).
\] (29.6.52)

As we know, the longitudinal field (potential) is screened and the physically relevant internal vector potential and field are
\[
A(q, \omega) = \frac{1}{\epsilon_r(q, \omega)} A_{\text{ext}}(q, \omega), \quad E(q, \omega) = \frac{1}{\epsilon_r(q, \omega)} E_{\text{ext}}(q, \omega).
\] (29.6.53)

Using (29.6.28) that relates the vector potential to the electric field we get
\[
j(q, \omega) = \frac{i}{\omega} \epsilon_r(q, \omega) \left[ P_\parallel(q, \omega) + \frac{n_e e^2}{m_e} \right] E(q, \omega),
\] (29.6.54)
from which
\[
\sigma_\parallel(q, \omega) = \frac{i}{\omega} \epsilon_r(q, \omega) \left[ P_\parallel(q, \omega) + \frac{n_e e^2}{m_e} \right].
\] (29.6.55)

The effect of screening appears in the factor \( \epsilon_r(q, \omega) \).

To get a simpler expression we rewrite the longitudinal conductivity in terms of the density–density response function. For that we multiply both sides of (29.6.52) by \( q \), rewrite the left-hand side in terms of the number density, and express the vector potential on the right-hand side by the scalar potential using (29.6.47). This leads to
\[
-\omega \langle n(q, \omega) \rangle = \left[ P_\parallel(q, \omega) + \frac{n_e e^2}{m_e} \right] \frac{q^2}{\omega} \varphi_{\text{ext}}(q, \omega).
\] (29.6.56)

On the other hand, the induced charge density and the external potential are related by the density–density response function \( \Pi(q, \omega) \). Comparing the above expression with (29.1.24) we find
\[
P_\parallel(q, \omega) + \frac{n_e e^2}{m_e} = \frac{\omega^2 e^2}{q^2} \Pi(q, \omega).
\] (29.6.57)

This relationship can be readily checked alternatively by evaluating the response functions directly. Using (29.1.31) and (29.6.26) and
\[ \langle \Psi_n | \mathbf{q} \cdot \hat{\mathbf{j}}(\mathbf{q}) | \Psi_m \rangle = \frac{e}{\hbar} (E_n - E_m) \langle \Psi_n | n(\mathbf{q}) | \Psi_m \rangle \]  

(29.6.58)

that follows from the continuity equation, we find

\[
\frac{\omega^2 e^2}{q^2} \Pi(\mathbf{q}, \omega) - P_\parallel(\mathbf{q}, \omega) = \frac{e^2}{\hbar^2 q^2} \frac{1}{V} \sum_{mn} \left( \frac{e^{-\beta E_n}}{Z} - \frac{e^{-\beta E_m}}{Z} \right) \times (\hbar \omega + E_m - E_n) \left| \langle \Psi_n | n(\mathbf{q}) | \Psi_m \rangle \right|^2
\]

\[
= \frac{e^2}{\hbar^2 q^2} \frac{1}{V} \sum_{mn} 2 \frac{e^{-\beta E_n}}{Z} (E_m - E_n) \left| \langle \Psi_n | n(\mathbf{q}) | \Psi_m \rangle \right|^2.
\]

On the other hand, the dynamical structure factor \(S(\mathbf{q}, \omega)\) is known to satisfy the sum rule [see (J.2.20)]

\[
\frac{1}{2\pi} \int_{-\infty}^{\infty} \omega S(\mathbf{q}, \omega) d\omega = \frac{\hbar q^2}{2m_e}.
\]

(29.6.60)

Substituting the spectral representation (28.4.92) into this equation, we find

\[
\frac{1}{\hbar N_e} \sum_{mn} \frac{e^{-\beta E_n}}{Z} (E_m - E_n) \left| \langle \Psi_n | n(\mathbf{q}) | \Psi_m \rangle \right|^2 = \frac{\hbar^2 q^2}{2m_e}.
\]

(29.6.61)

Combining this with (29.6.59) we in fact recover (29.6.57).

Inserting now (29.6.57) into (29.6.52) and using (29.6.28) valid for the longitudinal component, we find

\[
\hat{j}(\mathbf{q}, \omega) = -\frac{\omega^2 e^2}{q^2} \Pi(\mathbf{q}, \omega) A_{\text{ext}}(\mathbf{q}, \omega) = -\frac{\omega^2 e^2}{q^2} \Pi(\mathbf{q}, \omega) \epsilon(\mathbf{q}, \omega) A(\mathbf{q}, \omega)
\]

\[
= \frac{i\omega e^2}{q^2} \Pi(\mathbf{q}, \omega) \epsilon(\mathbf{q}, \omega) E(\mathbf{q}, \omega),
\]

(29.6.62)

from which we get

\[
\sigma(\mathbf{q}, \omega) = \frac{i\omega e^2}{q^2} \Pi(\mathbf{q}, \omega) \epsilon = \frac{i\omega e^2}{q^2} \tilde{\Pi}(\mathbf{q}, \omega).
\]

(29.6.63)

When (29.6.41) is applied to the longitudinal component,

\[
P_\parallel(\mathbf{q}, \omega) = \tilde{P}_\parallel(\mathbf{q}, \omega) + \tilde{S}_\parallel(\mathbf{q}, \omega) \frac{4\pi e^2 / q^2}{1 - (4\pi e^2 / q^2) \tilde{\Pi}(\mathbf{q}, \omega)} \tilde{S}(\mathbf{q}, \omega).
\]

(29.6.64)

The longitudinal current–density response function appearing here can be expressed using the continuity equation via the density–density response. We readily find

\[
S(\mathbf{q}, \omega) = -\frac{e \omega}{q} \Pi(\mathbf{q}, \omega).
\]

(29.6.65)
When it is written in terms of the irreducible parts, we have
\[
S_{\parallel}(q, \omega) = \tilde{S}_{\parallel}(q, \omega) + \tilde{S}_{\parallel}(q, \omega) \frac{4\pi \varepsilon_0^2 / q^2}{1 - (4\pi \varepsilon_0^2 / q^2) \tilde{\Pi}(q, \omega)} \tilde{\Pi}(q, \omega)
\]
\[
= \frac{\tilde{S}_{\parallel}(q, \omega)}{1 - (4\pi \varepsilon_0^2 / q^2) \tilde{\Pi}(q, \omega)},
\]
and hence
\[
\tilde{S}_{\parallel}(q, \omega) = -\frac{e \omega}{q} \tilde{\Pi}(q, \omega).
\]
Similar relations hold for the density–current response function. To check them we have to recognize that
\[
S_{\alpha}(q, \omega) = S_{\alpha}^*(q, \omega) |_{\delta \to -\delta},
\]
which follows from the spectral representations
\[
S_{\alpha}(q, \omega) = \frac{1}{V} \sum_{mn} \left( \frac{e^{-\beta E_n}}{Z} - \frac{e^{-\beta E_m}}{Z} \right) \frac{\langle \Psi_m | \hat{j}_\alpha(q) | \Psi_n \rangle}{h \omega - E_m + E_n + i\delta}.
\]
and
\[
\mathcal{S}_{\alpha}(q, \omega) = \frac{1}{V} \sum_{mn} \left( \frac{e^{-\beta E_n}}{Z} - \frac{e^{-\beta E_m}}{Z} \right) \frac{\langle \Psi_m | n(q) | \Psi_m \rangle}{h \omega - E_m + E_n + i\delta}.
\]
Since \(\Pi(q, \omega)\) itself satisfies the relation
\[
\Pi(q, \omega) = \Pi^*(q, \omega) |_{\delta \to -\delta},
\]
which can be best seen from the spectral representation in (29.1.31), we have
\[
\mathcal{S}_{\parallel}(q, \omega) = -\frac{e \omega}{q} \Pi(q, \omega).
\]
When this is written in terms of the irreducible parts we find
\[
\mathcal{S}_{\parallel}(q, \omega) = \mathcal{S}_{\parallel}(q, \omega) + \tilde{\Pi}(q, \omega) \frac{4\pi \varepsilon_0^2 / q^2}{1 - (4\pi \varepsilon_0^2 / q^2) \tilde{\Pi}(q, \omega)} \mathcal{S}_{\parallel}(q, \omega)
\]
\[
= \frac{\mathcal{S}_{\parallel}(q, \omega)}{1 - (4\pi \varepsilon_0^2 / q^2) \tilde{\Pi}(q, \omega)},
\]
and hence
\[
\mathcal{S}_{\parallel}(q, \omega) = -\frac{e \omega}{q} \tilde{\Pi}(q, \omega).
\]
Combining these expressions with (29.6.64) we find
\[
\tilde{P}_\parallel(q, \omega) + \frac{n_e e^2}{m_e} = \frac{\omega^2 e^2}{q^2} \tilde{\Pi}(q, \omega)
\]
\[
= \varepsilon(q, \omega) \left[ P_\parallel(q, \omega) + \frac{n_e e^2}{m_e} \right],
\]
which is equivalent to the statement that the longitudinal field is screened. When this relationship is used for the conductivity in (29.6.55) we get
\[
\sigma_\parallel(q, \omega) = \frac{i}{\omega} \left[ \tilde{P}_\parallel(q, \omega) + \frac{n_e e^2}{m_e} \right].
\]
Thus, indeed, it is the irreducible part of the current–current response that appears in the Kubo formula for the longitudinal conductivity.

29.6.4 Dielectric Tensor and Conductivity

It was mentioned in Chapter 16 that the conductivity and the dielectric constant are not independent of each other. Indeed (29.6.63) shows that the longitudinal conductivity can be expressed in terms of the irreducible density–density response function, which in turn is simply related to the dielectric function. We thus find
\[
\varepsilon_\parallel(q, \omega) = 1 + \frac{i}{\epsilon_0 \omega} \sigma_\parallel(q, \omega),
\]
which is exactly the relationship we have found in (16.1.64).

A similar equation holds for the transverse components. To derive it we combine Maxwell’s first equation (Ampère’s law) with Ohm’s law. The Maxwell equation is written either as
\[
\text{curl } B = \mu_0 \left( \epsilon_0 \frac{\partial E}{\partial t} + j \right)
\]
with the full electric-current density or as
\[
\text{curl } H = \frac{\partial D}{\partial t} + j_{\text{ext}},
\]
where only the external current appears on the right-hand side. The difference between the electric displacement and the electric field is due to the current \( j_{\text{ind}} \) induced by the electromagnetic field
\[
\frac{\partial D}{\partial t} = \epsilon_0 \frac{\partial E}{\partial t} + j_{\text{ind}}.
\]
Inserting (29.6.19) into (29.6.80) and using (29.1.5) we find
\[
\varepsilon_{\alpha\beta}(q, \omega) = \epsilon_0 \delta_{\alpha\beta} + \frac{i}{\omega} \sigma_{\alpha\beta}(q, \omega),
\]
which is nothing else than the generalization of (16.1.64). Thus the transverse component of the dielectric function and the transverse conductivity are related by

$$\epsilon_{\perp}(q, \omega) = 1 + \frac{i}{\epsilon_0 \omega} \sigma_{\perp}(q, \omega).$$  \hspace{1cm} (29.6.82)

### 29.6.5 Transverse Dielectric Function of the Electron Gas

An explicit expression can be derived for the transverse dielectric function by substituting (29.6.29) into (29.6.81). When the spectral representation of the current–current response function is used,

$$\epsilon_{\alpha\beta}(q, \omega) = \epsilon_0 \delta_{\alpha\beta} - \frac{1}{\omega^2} \left[ P_{\alpha\beta}(q, \omega) + \frac{n_e e^2}{m_e} \delta_{\alpha\beta} \right]$$

$$= \epsilon_0 \left( 1 - \frac{\omega p}{\omega^2} \right) \delta_{\alpha\beta} + \frac{i}{\omega^2} \frac{1}{V} \sum_{mn} \left( \frac{e^{-\beta E_n}}{Z} - \frac{e^{-\beta E_m}}{Z} \right) \langle \psi_n | \hat{j}_\alpha(q) | \psi_m \rangle \langle \psi_m | \hat{j}_\beta(-q) | \psi_n \rangle,$$

(29.6.83)

Choosing the propagation vector $q$ of the radiation field in the $z$-direction and calculating the response in the $x$-direction for free electrons, the transverse dielectric function has a form similar to the Lindhard function

$$\epsilon_{\perp}(q, \omega) = 1 - \frac{\omega_p^2}{\omega^2} - \frac{e^2}{\epsilon_0 m_e^2 \omega^2 \hbar^2 k_x^2} \sum_k \frac{f_0(\varepsilon_k) - f_0(\varepsilon_k + q)}{\hbar \omega - \varepsilon_{k+q} + \varepsilon_k + i\delta}.$$  \hspace{1cm} (29.6.84)

Comparison with (29.4.6) shows two differences between the formulas for the longitudinal and transverse components of the dielectric function. One is an extra term in the transverse component due to the diamagnetic current. The other is that the matrix element of the current appears in place of the dipole matrix element. We note that if the calculation is done for Bloch electrons, we find

$$\epsilon_{\perp}(q, \omega) = 1 - \frac{n_e e^2}{\epsilon_0 m_e \omega^2} - \frac{e^2}{\epsilon_0 m_e^2 \omega^2 \hbar^2 k_x^2} \sum_{knn'} \frac{f_0(\varepsilon_{nk}) - f_0(\varepsilon_{n'k+q})}{\hbar \omega - \varepsilon_{n'k+q} + \varepsilon_{nk} + i\delta} \times \left| \langle \psi_{n'k+q}^{(0)} | \frac{1}{2} \left( p_x e^{iqr} + e^{iqr} p_x \right) | \psi_{nk}^{(0)} \rangle \right|^2,$$

(29.6.85)

where the matrix element is

$$\langle \psi_{n'k+q}^{(0)} | \frac{1}{2} \left( p_x e^{iqr} + e^{iqr} p_x \right) | \psi_{nk}^{(0)} \rangle = \frac{1}{v_0} \int_{v_0} u_{n'k+q}^*(r) \frac{\hbar}{\imath} \nabla + \hbar \hat{k} + \frac{1}{2} \hbar q \right] u_{n,k}(r) \, dr.$$  \hspace{1cm} (29.6.86)

The transverse dielectric function can be calculated for free electrons in closed form. For the real part we have
\[ \epsilon_{1\perp}(q, \omega) = 1 - \frac{q^2}{q_F^2} \left\{ \frac{1}{8} \left( \frac{\hbar v_F q}{\hbar \omega} \right)^2 \left[ \left( \frac{\varepsilon_q}{\hbar v_F q} \right)^2 + 3 \left( \frac{\hbar \omega}{\hbar v_F q} \right)^2 + 1 \right] \right\} \]  

(29.6.87)

\[ - \frac{q}{4k_F} \left( \frac{\varepsilon_F}{\hbar \omega} \right)^2 \left\{ \left[ 1 - \left( \frac{\hbar \omega + \varepsilon_q}{\hbar v_F q} \right)^2 \right] \ln \left( \frac{\hbar \omega + \hbar v_F q + \varepsilon_q}{\hbar \omega - \hbar v_F q + \varepsilon_q} \right) \right. 

+ \left. \left[ 1 - \left( \frac{\hbar \omega - \varepsilon_q}{\hbar v_F q} \right)^2 \right] \ln \left( \frac{\hbar \omega - \hbar v_F q - \varepsilon_q}{\hbar \omega + \hbar v_F q - \varepsilon_q} \right) \right\} \right]. \]

The imaginary part is

\[ \epsilon_{2\perp}(q, \omega) = \begin{cases} 
\frac{\pi}{4} \frac{q v_F q}{\hbar} \left[ 1 - \left( \frac{\hbar \omega}{\hbar v_F q} \right)^2 - \left( \frac{\varepsilon_q}{\hbar v_F q} \right)^2 \right] 
for \ 0 \leq \hbar \omega < \hbar v_F q - \varepsilon_q, \\
\frac{\pi}{4} \frac{k_F q}{\hbar} \left( \frac{\varepsilon_F}{\hbar \omega} \right)^2 \left[ 1 - \left( \frac{\hbar \omega - \varepsilon_q}{\hbar v_F q} \right)^2 \right] \frac{q^2}{q_F^2} 
for \ \hbar v_F q - \varepsilon_q \leq \hbar \omega \leq \hbar v_F q + \varepsilon_q, \\
0 
for \ \hbar v_F q + \varepsilon_q \leq \hbar \omega.
\end{cases} \]  

(29.6.88)

\[ \epsilon_{2\perp}(q, \omega) = \begin{cases} 
0 
for \ 0 \leq \hbar \omega < \varepsilon_q - \hbar v_F q, \\
\frac{\pi}{4} \frac{k_F}{q} \left( \frac{\varepsilon_F}{\hbar \omega} \right)^2 \left[ 1 - \left( \frac{\hbar \omega - \varepsilon_q}{\hbar v_F q} \right)^2 \right] \frac{q^2}{q_F^2} 
for \ \varepsilon_q - \hbar v_F q \leq \hbar \omega \leq \varepsilon_q + \hbar v_F q, \\
0 
for \ \varepsilon_q + \hbar v_F q \leq \hbar \omega.
\end{cases} \]  

(29.6.89)

29.7 Optical and DC Conductivity

The formulas derived above will now be applied to calculate the conductivity in two special cases, at optical frequencies and in the limit \( \omega = 0 \), to get the optical and the DC conductivity, respectively.

29.7.1 Optical Conductivity

Since the momentum transfer during the emission or absorption of an optical photon is much less than the typical momenta of electrons in solids, the relevant quantities in the description of optical properties are the \( q \to 0 \) limits of the dielectric function and the conductivity. The real part of the quantity

\[ \sigma_{\perp}(\omega) = \lim_{q \to 0} \sigma_{\perp}(q, \omega) \]  

(29.7.1)
is called *optical conductivity*. It characterizes the response of the electron system to an electromagnetic radiation of frequency $\omega$. From the spectral representation of the Kubo formula [see (29.6.33)] we find

$$\text{Re} \sigma_\perp(\omega) = \frac{\pi}{\omega} \left(1 - e^{-\beta \omega}\right) \frac{1}{V} \sum_{mn} \frac{e^{-\beta E_n}}{Z} \left|\langle \Psi_n | \hat{j}_x | \Psi_m \rangle\right|^2 \delta(\hbar \omega - E_m + E_n).$$

(29.7.2)

This form allows a simple physical interpretation of the optical conductivity: It is the power absorbed from the electromagnetic field at frequency $\omega$.

An alternative, much used form of the Kubo formula, can be derived for the $q = 0$ component in uniform systems, if the current is written as the time derivative of the operator

$$Q = -e \sum_i r_i,$$

(29.7.3)

since

$$\dot{Q} = \frac{i}{\hbar} [H_0, Q] - \frac{e}{m_e} \sum_i p_i = \hat{j}.$$

(29.7.4)

Using this in (29.6.30) we find

$$\sigma_{\alpha\beta}(\omega) = \frac{1}{\hbar \omega V} \int_0^\infty dt \frac{e^{i(\omega+i\delta)t}}{\omega} \frac{d}{dt} \left\langle [Q_\alpha(t), \hat{j}_\beta(0)]_- \right\rangle + \frac{i e^2}{m_e \omega} \delta_{\alpha\beta},$$

(29.7.5)

which after integration by parts yields

$$\sigma_{\alpha\beta}(\omega) = -\frac{i}{\hbar V} \int_0^\infty dt \frac{e^{i(\omega+i\delta)t}}{\omega} \left\langle [Q_\alpha(t), \hat{j}_\beta(0)]_- \right\rangle$$

(29.7.6)

$$- \frac{1}{\hbar \omega V} \left\langle [Q_\alpha(0), \hat{j}_\beta(0)]_- \right\rangle + \frac{i e^2}{m_e \omega} \delta_{\alpha\beta}.$$

Making use of the canonical commutation relations we find

$$[Q_\alpha(0), \hat{j}_\beta(0)]_- = \frac{i \hbar e^2 N_e}{m_e}.$$

(29.7.7)

Hence the second and third terms cancel each other exactly. The thermal average in the first term can be written in terms of the equilibrium density matrix $\rho_0 = e^{-\beta H}/Z$ of the unperturbed system. After a cyclic permutation of the operators in the trace

$$\sigma_{\alpha\beta}(\omega) = -\frac{i}{\hbar V} \int_0^\infty dt \frac{e^{i(\omega+i\delta)t}}{\omega} \text{Tr} \left( \rho_0 [Q_\alpha(t), \hat{j}_\beta(0)]_- \right)$$

(29.7.8)

$$= \frac{i}{\hbar V} \int_0^\infty dt \frac{e^{i(\omega+i\delta)t}}{\omega} \text{Tr} \left( [Q_\alpha(t), \rho_0]_- \hat{j}_\beta(0) \right).$$
This expression can be further manipulated by using the operator identity

\[ e^{\beta \mathcal{H}_0} A(t) e^{-\beta \mathcal{H}_0} = \frac{1}{\hbar} \int_0^{\beta \hbar} d\lambda e^{\lambda \mathcal{H}_0 / \hbar} [\mathcal{H}_0, A(t)] e^{-\lambda \mathcal{H}_0 / \hbar} \]

which is equivalent to

\[ [A(t), \rho_0] = -i \rho_0 \int_0^{\beta \hbar} d\lambda \hat{A}(t - i\lambda), \quad (29.7.10) \]

where \( \hat{A} \) denotes the time derivative of \( A \). Applying this transformation in (29.7.8) and taking into account that the derivative of \( Q \) is the current, we find

\[ \sigma_{\alpha\beta}(\omega) = \frac{1}{\hbar V} \int_0^\infty dt \int_0^{\beta \hbar} d\lambda e^{i(\omega + i\delta)t} \langle \hat{j}_\alpha(t - i\lambda) \rangle \langle \hat{j}_\beta(0) \rangle, \quad (29.7.11) \]

or after a rearrangement of the operators

\[ \sigma_{\alpha\beta}(\omega) = \frac{1}{\hbar V} \int_0^\infty dt \int_0^{\beta \hbar} d\lambda e^{i(\omega + i\delta)t} \langle \hat{j}_\beta(-i\lambda) \hat{j}_\alpha(t) \rangle. \quad (29.7.12) \]

### 29.7.2 Optical Conductivity of the Electron Gas

We note that in the long-wavelength \( (q \to 0) \) limit, when there is no preferred direction in an isotropic system, the longitudinal and transverse components of the dielectric function and of the conductivity become identical,

\[ \epsilon_\parallel(0, \omega) = \epsilon_\perp(0, \omega) \quad \text{and} \quad \sigma_\parallel(0, \omega) = \sigma_\perp(0, \omega). \quad (29.7.13) \]

We will therefore use the expressions derived for the longitudinal component of the conductivity tensor given in (29.6.63), although, strictly speaking, the optical conductivity is related to the transverse response. In the RPA \( \tilde{\Pi} \) is replaced with \( \Pi_0 \). Looking at (29.2.46) we see that

\[ \Pi_0(q, \omega) = \frac{2}{V} \sum_k f_0(\varepsilon_k) \frac{2(\varepsilon_k + q - \varepsilon_k)}{(\hbar \omega + i\delta)^2 - (\varepsilon_k + q - \varepsilon_k)^2}, \quad (29.7.14) \]

from which in the \( v_F q \ll \omega \) limit we obtain
\[ \Pi_0(\mathbf{q}, \omega) \approx \frac{n_e q^2}{m_e \omega^2}. \]  

(29.7.15)

Inserting this expression into (29.6.63) gives

\[ \sigma(\omega) = i \frac{n_e e^2}{m_e \omega}. \]  

(29.7.16)

As it stands, a purely imaginary conductivity with no real part cannot be true; it does not satisfy the Kramers–Kronig relations. Assuming that the above form is valid for the imaginary part, the Kramers–Kronig relations give vanishing real part at nonzero frequencies, but a finite, singularly large value at \( \omega = 0 \):

\[ \text{Re} \sigma(\omega) = \pi \frac{n_e e^2}{m_e} \delta(\omega). \]  

(29.7.17)

This sharp peak in the real part of the conductivity is the Drude peak. The real and imaginary parts can be combined into the expression

\[ \sigma(\omega) = i \frac{n_e e^2}{m_e (\omega + i \delta)}. \]  

(29.7.18)

One can show that this expression is valid more generally whenever scattering by lattice vibrations or by impurities can be neglected, and only the electron–electron interaction is taken into account since then energy is not dissipated in the system.

The finite lifetime of electron states due to scattering by impurities or lattice vibrations will modify this situation. According to (29.2.89) \( \tilde{\Pi} \) can be approximated by

\[ \tilde{\Pi}(\mathbf{q}, \omega) = \frac{n_e q^2}{m_e \omega (\omega + i/\tau)}, \]  

(29.7.19)

which leads to the result known from the Drude model

\[ \sigma(\omega) = i \frac{n_e e^2}{m_e (\omega + i/\tau)} = \frac{n_e e^2 \tau}{m_e (1 - i\omega \tau)}, \]  

(29.7.20)

and

\[ \text{Re} \sigma(\omega) = \frac{n_e e^2 \tau}{m_e} \frac{1}{1 + (\omega \tau)^2} = \frac{\sigma_0}{1 + (\omega \tau)^2}. \]  

(29.7.21)

The Drude peak is broadened by the scattering processes, the width is proportional to \( 1/\tau \), and the optical conductivity decays as \( 1/\omega^2 \) for high frequencies:

\[ \text{Re} \sigma(\omega) \approx \frac{n_e e^2}{m_e \omega^2 \tau}. \]  

(29.7.22)

This form of frequency-dependent conductivity satisfies the *conductivity sum rule*.
$$\int_0^\infty d\omega \, \text{Re} \sigma(\omega) = \frac{\pi n_e e^2}{2m_e}$$  \hspace{1cm} (29.7.23)\)

derived in (J.2.11).

When a more realistic band structure is considered, photons can be absorbed or emitted in association with interband transitions in the electron system. Thus, as has been discussed in Chapter 25, the imaginary part of the dielectric function and hence the optical conductivity gives information about the joint density of states of the bands between which the transition takes place. The Van Hove singularities of the joint density of states produce sharp structures in $\sigma(\omega)$. Similar sharp features may appear in the dielectric function and optical conductivity at frequencies corresponding to the absorption or emission of optical phonons. Nevertheless, the optical $f$-sum rule has to be satisfied.

Note that if the transverse response is studied, the contribution given in (29.7.16) and hence the Drude peak arises from the diamagnetic term. Its contribution to the real part of the conductivity is singular and proportional to $\delta(\omega)$, even when scattering processes are taken into account. This singularity is, however, unphysical. By considering the properties of the irreducible current–current response function one can show that its real part cancels exactly the contribution of the diamagnetic term in the $\omega \to 0$ limit, and the imaginary part is proportional to $\omega$. This then leads to a finite conductivity even at $\omega = 0$.

### 29.7.3 DC Conductivity

The DC conductivity is obtained by taking the limit $q \to 0$ first and the limit $\omega \to 0$ afterward in (29.6.33). Using the relationship

$$\lim_{\omega \to 0} \frac{1}{\omega} \left(1 - e^{-\beta \hbar \omega}\right) = \beta \hbar,$$  \hspace{1cm} (29.7.24)

we have

$$\text{Re} \sigma_{\alpha\beta} = \frac{1}{2k_B T V} \int_{-\infty}^\infty \frac{1}{\omega} \langle \hat{j}_\alpha(t)\hat{j}_\beta \rangle \; \text{d}t,$$  \hspace{1cm} (29.7.25)

$$= \frac{\pi \hbar}{k_B T V} \sum_{mn} \frac{e^{-\beta E_n}}{Z} \langle \Psi_n | \hat{j}_\alpha | \Psi_m \rangle \langle \Psi_m | \hat{j}_\beta | \Psi_n \rangle \delta(E_m - E_n).$$

\footnote{We note that the order of the limits is different when the static dielectric constant or the static magnetic susceptibility is calculated. The limit $\omega \to 0$ has to be performed first for finite $q$, and only after that we can take the limit $q \to 0$. Otherwise the Lindhard function gives zero, because the number of particles and the magnetization are conserved quantities.}
Although (29.7.25) is a seemingly simple expression, the explicit calculation of the conductivity using this formula is not easy and has only been done in a few simple cases. The difficulties, which are related to the fact that it does not suffice to carry out the calculations in some low orders of perturbation theory, can be readily seen when scattering by impurities is considered.

According to the lowest order Born approximation the inverse collision time is proportional to the absolute square of the matrix element of the scattering potential $V_{\text{imp}}$:

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} n_i \rho(\varepsilon_F) |V_{\text{imp}}|^2,$$

(29.7.26)

where $n_i$ is the concentration of impurities. Thus, a second-order calculation of the current–current response would give a conductivity that is inversely proportional to the collision time. We know, however, that according to the celebrated Drude formula

$$\sigma = \frac{n_e e^2 \tau}{m_e},$$

(29.7.27)

the conductivity is proportional to the collision time of electrons. This result can be obtained in a perturbative treatment of the response function only if the contribution of the scattering processes are summed up to infinite order. A partial summation can be achieved by including a finite lifetime for the propagating electrons and holes when calculating the current–current response function. This approximation corresponds to taking into account the so-called self-energy corrections, but neglecting the processes that would directly or indirectly couple the electron and the hole. When the form

$$G_R(k, \omega) = \frac{1}{\hbar \omega - \varepsilon_k + i\hbar/2\tau},$$

(29.7.28)

is used for the retarded Green function, we obtain

$$\tilde{P}_{\alpha\alpha} = -\frac{n_e}{m_e} \frac{1}{1 - i\omega/\tau},$$

(29.7.29)

for the response function. This would yield a Drude-like expression for the conductivity with this $\tau$ as the relaxation time. This result is, however, still not correct. To describe the contribution of the scattering processes to the conductivity properly, the so-called vertex corrections have to be taken into account as well. To understand their role we recall that the correct expression for the conductivity contains the so-called transport relaxation time, which differs from the usual lifetime of electrons. The scattering processes are weighted by a factor $1 - \cos \theta$, where $\theta$ is the change in the direction of the scattered electron, when the transport relaxation time is calculated. This factor takes into account the effectiveness of losing current due to scattering.
29.7.4 The Kubo–Greenwood Formula

A more convenient, simpler, and, in some cases, more easily applicable expression can be obtained by the following considerations: We neglect the diamagnetic term since it gives contribution only to the imaginary part and

\[
\hat{j} = -e \frac{\hbar}{i m_e V} \sum_{i=1}^{N_e} \nabla_i \tag{29.7.30}
\]

is used for the current operator, while the interaction with the electromagnetic field is expressed in terms of the electric field instead of the vector potential in the form

\[
\mathcal{H}_{\text{ext}} = - \frac{\hbar e}{m_e \omega} \sum_{i=1}^{N_e} E \cdot \nabla_i. \tag{29.7.31}
\]

To calculate the expectation value of the current we start from

\[
j = \langle \hat{j} \rangle = \text{Tr} \left\{ \rho^{(1)} \hat{j} \right\}, \tag{29.7.32}
\]

where \( \rho^{(1)} \) is the first-order correction to the density matrix due to the interaction with the electromagnetic field. According to (J.1.35)

\[
\rho^{(1)}(t) = \frac{i}{\hbar} \int_{-\infty}^{t} e^{-i\mathcal{H}_0(t-t')/\hbar} [\rho_0, \mathcal{H}_{\text{ext}}(t')] e^{i\mathcal{H}_0(t-t')/\hbar} \delta t'. \tag{29.7.33}
\]

The trace in (29.7.32) is evaluated using a complete set of many-body eigenstates \( |\Psi_n \rangle \). Insertion of a complete set of intermediate states gives

\[
j = \sum_{mn} \langle \Psi_n | \hat{j} | \Psi_m \rangle \langle \Psi_m | \rho^{(1)} | \Psi_n \rangle. \tag{29.7.34}
\]

The matrix elements of the current are obtained from (29.7.30), while the matrix elements of the density matrix can be evaluated using (29.7.33). For its temporal Fourier transform we find

\[
\langle \Psi_m | \rho^{(1)} | \Psi_n \rangle = \left( \frac{e^{-\beta E_n}}{Z} - \frac{e^{-\beta E_m}}{Z} \right) \frac{\langle \Psi_m | \mathcal{H}_{\text{ext}} | \Psi_n \rangle}{\hbar \omega - E_m + E_n + i\delta}. \tag{29.7.35}
\]

In the one-electron approximation the many-body states are Slater determinants built up from single-particle functions \( \varphi_n \) of energy \( \varepsilon_n \). The real part of the conductivity then takes the form

\[
\text{Re} \sigma_{\alpha\beta} = \frac{\pi e^2 \hbar^2}{m_e^2 \omega V} \sum_{mn} \left[ f_0(\varepsilon_m) - f_0(\varepsilon_n) \right] \langle \varphi_n | \nabla_\alpha | \varphi_m \rangle \langle \varphi_m | \nabla_\beta | \varphi_n \rangle \delta(\varepsilon_m - \varepsilon_n - \hbar \omega), \tag{29.7.36}
\]

\[
\times \langle \varphi_n | \nabla_\alpha | \varphi_m \rangle \langle \varphi_m | \nabla_\beta | \varphi_n \rangle \delta(\varepsilon_m - \varepsilon_n - \hbar \omega), \tag{29.7.36}
\]
where \( f_0 \) is the Fermi distribution function. Assuming that the matrix element can be approximated by an average matrix element depending only on the energy of the state, the summation over the states can be converted to an integral over energy where the density of states appears in the integrand:

\[
\text{Re} \sigma_{\alpha\beta} = \frac{\pi e^2 \hbar^2}{m_e^2 \omega} \int d\varepsilon \rho(\varepsilon) \rho(\varepsilon + \hbar \omega) \left[ f_0(\varepsilon + \hbar \omega) - f_0(\varepsilon) \right] \\
\times \langle \varphi_{\varepsilon} \nabla_{\alpha} | \varphi_{\varepsilon + \hbar \omega} \rangle \langle \varphi_{\varepsilon + \hbar \omega} | \nabla_{\beta} | \varphi_{\varepsilon} \rangle.
\] (29.7.37)

In the static, \( \omega \rightarrow 0 \) limit, the difference between the Fermi distribution functions is replaced by the derivative \( \partial f_0 / \partial \varepsilon \). Finally, in isotropic systems, the DC conductivity can be written in the form

\[
\sigma = - \int \sigma_\varepsilon(0) \frac{\partial f_0}{\partial \varepsilon} d\varepsilon,
\] (29.7.38)

where

\[
\sigma_\varepsilon(0) = \frac{\pi e^2 \hbar^2}{m_e^2} \left[ \rho(\varepsilon) \right]^2 \left| \left< \varphi_{\varepsilon} \right| \frac{\partial}{\partial x} \left| \varphi_{\varepsilon} \right> \right|^2.
\] (29.7.39)

This is the *Kubo–Greenwood formula*.\(^10\) Besides the density of states the conductivity is determined by the matrix element of the operator \( \partial / \partial x \). As expected on physical grounds and expressed mathematically by the factor \( -\partial f_0 / \partial \varepsilon \), only electrons lying in the neighborhood of the Fermi energy in a range of width \( k_B T \) contribute to the integral. Thus it suffices to know the wavefunction of states near the Fermi energy.

The situation is different in semiconductors. The states responsible for conduction are at the bottom of the conduction band or at the top of the valence band, typically much farther away from the chemical potential than \( k_B T \), i.e., \( \varepsilon - \mu \gg k_B T \) for electrons in the conduction band. In this limit classical statistics can be used instead of Fermi statistics and

\[
\frac{\partial f_0(\varepsilon)}{\partial \varepsilon} \approx - \frac{f_0(\varepsilon)}{k_B T}.
\] (29.7.40)

The conductivity can then be written in the form

\[
\sigma = e \int \mu(\varepsilon) n(\varepsilon) d\varepsilon,
\] (29.7.41)

where

\[
\mu(\varepsilon) = \frac{\sigma_\varepsilon(0)}{e k_B T \rho(\varepsilon)}
\] (29.7.42)

is the mobility and

\[
n(\varepsilon) = \rho(\varepsilon) f_0(\varepsilon)
\] (29.7.43)

\(^{10}\) D. A. Greenwood, 1958.
is the density of electrons. If $\sigma_\varepsilon$ vanishes for $\varepsilon < \varepsilon_c$, and this is the case for extrinsic $n$-type semiconductors, there are no mobile charge carriers below the conduction band. The conductivity then has an activated form

$$\sigma \approx \sigma_\varepsilon e^{-(\varepsilon_c - \mu)/k_B T}. \quad (29.7.44)$$

A similar activated form is obtained for disordered systems if the electron states near the Fermi energy are localized and do not contribute to the conduction.

29.8 Response to Magnetic Perturbations

The external perturbations considered until now couple identically to electrons of both spin orientations and give rise to a change in the electronic density or generate a current. An external magnetic field couples to the magnetic-moment density acting oppositely on electrons of opposite spin and results in a net magnetization when the field is homogeneous in space. For weak enough disturbance the response to the magnetic field is linear in the field strength, and the proportionality factor is the magnetic susceptibility. Because this response depends on the internal dynamics of the system, the magnetic susceptibility, like the dielectric function, is sensitive to the electron–electron interaction. We will first calculate how, in a simple Hubbard model of interacting electrons, the Pauli susceptibility is modified by this interaction. Then the dynamical susceptibility will be studied. Finally, the Ruderman–Kittel oscillations, the magnetic analog of the Friedel oscillations, will be considered.

29.8.1 Stoner Enhancement of the Susceptibility

The dielectric response of the electron gas was calculated analytically for electrons moving in a uniform neutralizing background, interacting with each other by Coulomb repulsion. In this model, as will be seen in Chapter 30, magnetic fluctuations are weak at the usual metallic densities. Magnetic instability may appear only at very low densities, for large values of $r_s$. To get a more realistic picture of the magnetic properties of metals we should consider electrons in $d$ or $f$ states rather than free electrons. Such electrons can reasonably be described in the tight-binding approximation, and a Hubbard-like model may be more appropriate. We will therefore study the influence of electron–electron interaction on the susceptibility in the Hubbard model.

The Hartree–Fock theory of the Hubbard model was presented in the previous chapter. We saw that the quasiparticle energies are

$$\tilde{\varepsilon}_{k\sigma} = \varepsilon_k + U \langle n_{-\sigma} \rangle, \quad (29.8.1)$$

where the average number of particles with spin $\sigma$ and per unit volume has to be determined self-consistently from
\[ \langle n_\sigma \rangle = \frac{1}{V} \sum_k \langle n_{k\sigma} \rangle = \frac{1}{V} \sum_k f_0(\tilde{\varepsilon}_{k\sigma}). \]  \hfill (29.8.2)

When an external field \( \mathbf{H} \) is applied, an additional spin-dependent shift appears in the single-particle energies. Choosing the quantization axis in the direction of the field, the quasiparticle energies are modified to

\[ \tilde{\varepsilon}_{k\uparrow} = \varepsilon_k + U \langle n_\downarrow \rangle - \frac{1}{2} g_e \mu_B \mu_0 H, \quad \tilde{\varepsilon}_{k\downarrow} = \varepsilon_k + U \langle n_\uparrow \rangle + \frac{1}{2} g_e \mu_B \mu_0 H, \]  \hfill (29.8.3)

where the densities \( \langle n_\uparrow \rangle \) and \( \langle n_\downarrow \rangle \) have to be determined self-consistently for a fixed total electron density

\[ n_e = \frac{N_e}{V} = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle. \]  \hfill (29.8.4)

The magnetization is obtained from the difference of the number of particles with up- and down-spin orientations:

\[ M = \frac{1}{2} g_e \mu_B [\langle n_\uparrow \rangle - \langle n_\downarrow \rangle] = \frac{1}{2} g_e \mu_B \frac{1}{V} \sum_k [\langle n_{k\uparrow} \rangle - \langle n_{k\downarrow} \rangle] \]

\[ = \frac{1}{2} g_e \mu_B \frac{1}{V} \sum_k [f_0(\tilde{\varepsilon}_{k\uparrow}) - f_0(\tilde{\varepsilon}_{k\downarrow})]. \]  \hfill (29.8.5)

For weak magnetic fields the Fermi distribution functions can be expanded to linear order in the energy correction yielding

\[ M = \frac{1}{2} g_e \mu_B \frac{1}{V} \sum_k \frac{\partial f_0(\varepsilon_k)}{\partial \varepsilon} [U \langle n_\downarrow \rangle - \frac{1}{2} g_e \mu_B \mu_0 H - U \langle n_\uparrow \rangle - \frac{1}{2} g_e \mu_B \mu_0 H]. \]  \hfill (29.8.6)

Replacing the summation by an integral, we find

\[ M = \frac{1}{2} g_e \mu_B \int \frac{\partial f_0(\varepsilon)}{\partial \varepsilon} [U \langle n_\downarrow \rangle - U \langle n_\uparrow \rangle - g_e \mu_B \mu_0 H] \rho_\sigma(\varepsilon) \, d\varepsilon, \]  \hfill (29.8.7)

where \( \rho_\sigma(\varepsilon) \) is the density of states for one spin orientation. At low temperatures, where the thermal corrections in the Sommerfeld expansion can be neglected, the leading term gives

\[ M = -\frac{1}{2} g_e \mu_B [U \langle n_\downarrow \rangle - U \langle n_\uparrow \rangle - g_e \mu_B \mu_0 H] \rho_\sigma(\varepsilon_F). \]  \hfill (29.8.8)

The quantity \( \langle n_\uparrow \rangle - \langle n_\downarrow \rangle \) on the right-hand side can be expressed by the magnetization using (29.8.5). We then find

\[ M = U \rho_\sigma(\varepsilon_F) M + \frac{1}{2} g_e^2 \mu_B^2 \mu_0 \rho_\sigma(\varepsilon_F) H, \]  \hfill (29.8.9)

from which

\[ M = \frac{\frac{1}{2} g_e^2 \mu_B^2 \mu_0 \rho_\sigma(\varepsilon_F)}{1 - U \rho_\sigma(\varepsilon_F)} H. \]  \hfill (29.8.10)
The susceptibility is then

\[ \chi = \frac{1}{2} g_\sigma^2 \mu_0^2 \mu B_\mu \rho \sigma (\varepsilon_F) \left( 1 - U \rho \sigma (\varepsilon_F) \right). \]  

(29.8.11)

The expression in the numerator is just the Pauli susceptibility of the free-electron gas derived in (16.2.113). Coulomb repulsion gives rise to its increase through the factor \( S = 1/[1 - U \rho \sigma (\varepsilon_F)] \) which is known as the Stoner enhancement factor.\(^{11}\)

The unpolarized, paramagnetic state, where \( \tilde{\varepsilon}_{k \uparrow} = \tilde{\varepsilon}_{k \downarrow} \) and \( \langle n_\uparrow \rangle = \langle n_\downarrow \rangle \), is stable without external magnetic field, if \( U \rho \sigma (\varepsilon_F) < 1 \). The Stoner factor is positive and the susceptibility is indeed enhanced. When the interaction is strong enough or the density of states is large, the paramagnetic state becomes unstable even without external magnetic field. A polarized, ferromagnetic state may appear in which the equality of the number of electrons with opposite spin orientations is broken spontaneously. The condition \( U \rho \sigma (\varepsilon_F) = 1 \) obtained for this transition in the mean-field approximation is, however, only a rough estimate. Transition to a homogeneous magnetic state cannot so easily occur when correlations between electrons are taken into account. Without going into these details we will study the properties of the broken-symmetry state in Chapter 33.

Materials in which the symmetry is not broken spontaneously but \( U \rho \sigma (\varepsilon_F) \) is close to the instability threshold are of particular interest. Being close to the threshold where the system becomes ferromagnetic, these metals are called nearly ferromagnetic. As indicated by the large Stoner enhancement factor, magnetic fluctuations are strongly enhanced in them and they give rise to modifications in the thermodynamic properties (e.g., the temperature dependence of the specific heat) compared to ordinary metals. Among the elemental metals platinum and palladium fall into this class. The best estimate for palladium is \( U \rho \sigma (\varepsilon_F) \approx 0.9 \).

29.8.2 Dynamical Susceptibility

Having determined the static susceptibility we now turn to the problem where a weak, spatially and temporally varying magnetic field \( H_{\text{ext}}(r, t) \) is applied to the system in addition to a stronger uniform, static magnetic field \( H \). The uniform field shifts the one-particle energies of up- and down-spin electrons oppositely and gives rise to a spatially uniform magnetization. We will study how the magnetization is modified by the weak oscillating field.

Assuming that the weak field can be treated as a perturbation, the perturbation Hamiltonian is

\[ \text{\footnotesize \cite{Stoner1938}} \]

\(^{11}\) E. C. Stoner, 1938.
Electronic Response to External Perturbations

\[ \mathcal{H}_1(t) = -\mu_0 \int H_{\text{ext}}(r, t) \cdot \mathbf{m}(r) \, dr \]

\[ = -\frac{\mu_0}{V} \sum_q H_{\text{ext}}(q, t) \cdot \mathbf{m}(-q), \quad (29.8.12) \]

where \( \mathbf{m}(r) \) is the operator of the magnetic-moment density, its expectation value is the local magnetization, and \( \mathbf{m}(q) \) is its Fourier transform. For simplicity we assume that the perturbing field varies in space and time with wave vector \( q \) and frequency \( \omega \). In response to this perturbation a magnetization component appears that has the same wave vector and frequency:

\[ \langle \mathbf{m}(q, \omega) \rangle = \chi(q, \omega) H_{\text{ext}}(q, \omega), \quad (29.8.13) \]

where \( \chi(q, \omega) \) is the dynamical susceptibility. It follows from linear response theory that apart from a factor \( \mu_0 \) the components of the susceptibility tensor are the temporal Fourier transforms of the magnetization–magnetization response function:

\[ \chi_{\alpha\beta}(q, t - t') = \frac{i}{\hbar} \mu_0 \theta(t - t') \frac{1}{V} \left[ \mathbf{m}^\alpha(q, t), \mathbf{m}^\beta(-q, t') \right]_-. \quad (29.8.14) \]

This equation is the analog of the relationship between the electrical polarizability and the density–density response function.

Choosing the weak frequency-dependent field in the same (z) direction as the uniform field, the parallel (longitudinal) susceptibility is defined by

\[ \chi_\parallel(q, \omega) = \frac{\langle m_z(q, \omega) \rangle}{H_{\text{ext}}(q, \omega)}, \quad (29.8.15) \]

This response function is obtained by using the \( z \)-component of the magnetic-moment density in (29.8.14):

\[ \chi_\parallel(q, t - t') = \frac{i}{\hbar} \mu_0 \theta(t - t') \frac{1}{V} \left[ m_z(q, t), m_z(-q, t') \right]_. \quad (29.8.16) \]

When the spin density is used instead of the magnetic-moment density, we have

\[ \chi_\parallel(q, \omega) = \frac{g_e B}{H_{\text{ext}}(q, \omega)}, \quad (29.8.17) \]

and accordingly

\[ \chi_\parallel(q, \omega) = g^2_e B^2 \mu_0 \Sigma_\parallel(q, \omega), \quad (29.8.18) \]

where \( \Sigma_\parallel(q, \omega) \) is the Fourier transform of the spin-density response function:

\[ \Sigma_\parallel(q, \omega) = \frac{i}{\hbar} \int_0^\infty \text{d}(t - t') e^{i\omega(t - t') - \delta(t - t')} \frac{1}{V} \left[ s_z(q, t), s_z(-q, t') \right]_. \quad (29.8.19) \]
The magnetization–magnetization response function is a retarded Green function and as such it can be calculated using the methods of many-body theory. In principle, one should sum up all processes to all orders of perturbation theory. Here we will apply the much simpler equation-of-motion method described in Appendix J. We will study how the expectation value of \( s^z(q, \omega) \) changes due to the external perturbation.

If the magnetization is written in second-quantized form using (H.2.62), its Fourier transform is

\[
m(q) = \frac{1}{2} g_e \mu_B \sum_{k \alpha \beta} c^\dagger_{k \alpha} \sigma_{\alpha \beta} c_{k+q \beta},
\]

(29.8.20)

where \( \sigma \) is the Pauli matrix and the spin density is

\[
s(q) = \frac{1}{2} \sum_{k \alpha \beta} c^\dagger_{k \alpha} \sigma_{\alpha \beta} c_{k \beta}.
\]

(29.8.21)

The component along the quantization axis is

\[
s^z(q, t) = \frac{1}{2} [n^\uparrow(q, t) - n^\downarrow(q, t)]
= \frac{1}{2} \sum_k \left[ c^\dagger_{k \uparrow}(t) c_{k+q \uparrow}(t) - c^\dagger_{k \downarrow}(t) c_{k+q \downarrow}(t) \right].
\]

(29.8.22)

The equation of motion will be written separately for \( n^\uparrow(q, t) \) and \( n^\downarrow(q, t) \) using

\[
\mathcal{H}_1 = -\frac{1}{2} g_e \mu_B \mu_0 \frac{1}{V} \sum_{k q} H^z_{\text{ext}}(q, t) \left[ c^\dagger_{k+q \uparrow} c^\dagger_{k \uparrow} - c^\dagger_{k+q \downarrow} c^\dagger_{k \downarrow} \right]
\]

(29.8.23)

as perturbation.

If, for the sake of simplicity, the on-site Coulomb repulsion of the Hubbard model is used to describe the interaction between electrons, then

\[
\left( -\frac{\hbar}{i} \frac{d}{dt} + \varepsilon_{k \uparrow} \right) c^\dagger_{k \uparrow}(t) = -\frac{U}{V} \sum_{k' q'} c^\dagger_{k' - q' \downarrow}(t) c^\dagger_{k+q' \uparrow}(t) c_{k' \downarrow}(t) c_{k+q' \uparrow}(t)

\]

(29.8.24)

\[
+ \frac{1}{2} g_e \mu_B \mu_0 \frac{1}{V} \sum_{q'} H^z_{\text{ext}}(q', t) c^\dagger_{k+q' \uparrow}(t),
\]

\[
\left( -\frac{\hbar}{i} \frac{d}{dt} + \varepsilon_{k \downarrow} \right) c^\dagger_{k \downarrow}(t) = -\frac{U}{V} \sum_{k' q'} c^\dagger_{k' - q' \uparrow}(t) c^\dagger_{k+q' \downarrow}(t) c_{k' \uparrow}(t) c_{k+q' \downarrow}(t)

\]

(29.8.25)

\[-\frac{1}{2} g_e \mu_B \mu_0 \frac{1}{V} \sum_{q'} H^z_{\text{ext}}(q', t) c^\dagger_{k+q' \downarrow}(t),
\]
\[
\left(-\frac{\hbar}{i}\frac{d}{dt} - \varepsilon_{k + q}\right) c_{k+q\uparrow}(t) = \frac{U}{V} \sum_{k'q'} c_{k'\uparrow-q'\downarrow}(t)c_{k'\downarrow}(t)c_{k+q-q'\uparrow}(t) \tag{29.8.26}
\]
\[
-\frac{1}{2} g_{e}\mu_{B} \mu_{0} \frac{1}{V} \sum_{q'} H_{\text{ext}}^{z}(q', t) c_{k+q-q'\uparrow}(t),
\]
\[
\left(-\frac{\hbar}{i}\frac{d}{dt} - \varepsilon_{k+q}\right) c_{k+q\downarrow}(t) = \frac{U}{V} \sum_{k'q'} c_{k'\uparrow-q'\downarrow}(t)c_{k'\downarrow}(t)c_{k+q-q'\uparrow}(t) \tag{29.8.27}
\]
\[
+\frac{1}{2} g_{e}\mu_{B} \mu_{0} \frac{1}{V} \sum_{q'} H_{\text{ext}}^{z}(q', t) c_{k+q-q'\uparrow}(t).
\]

These equations can be linearized if the product \(c_{k'\uparrow-q'\sigma}(t)c_{k'\sigma}(t)\) appearing on the right-hand side in the terms containing three operators is replaced with its expectation value. In doing so we have to take into account that the quantity \(\langle c_{k'\uparrow-q'\sigma}(t)c_{k'\sigma}(t)\rangle\) is finite only if \(q' = 0\) or \(q'\) is equal to the wave vector of the external perturbing field. The term with \(q' = 0\) gives the Hartree correction of the one-particle energies. That is why \(\tilde{\varepsilon}_{k\sigma}\) and \(\tilde{\varepsilon}_{k+q\sigma}\) appear in the equations below instead of \(\varepsilon_{k\sigma}\) and \(\varepsilon_{k+q\sigma}\). By a change of variables \(k' \to k' + q\) in the summation and combining the above equations we find

\[
\left(-\frac{\hbar}{i}\frac{d}{dt} - \tilde{\varepsilon}_{k+q\uparrow} + \tilde{\varepsilon}_{k\uparrow}\right) \langle c_{k\uparrow}(t)c_{k+q\downarrow}(t) \rangle
\]
\[
= -\frac{U}{V} \sum_{k'} \langle c_{k'\downarrow}(t)c_{k'\uparrow}(t)\rangle \left[ f_{0}(\tilde{\varepsilon}_{k+q\uparrow}) - f_{0}(\tilde{\varepsilon}_{k\uparrow}) \right] \tag{29.8.28}
\]
\[
+\frac{1}{2} g_{e}\mu_{B} \mu_{0} H_{\text{ext}}^{z}(q, t) \frac{1}{V} \left[ f_{0}(\tilde{\varepsilon}_{k+q\uparrow}) - f_{0}(\tilde{\varepsilon}_{k\uparrow}) \right],
\]
\[
\left(-\frac{\hbar}{i}\frac{d}{dt} - \tilde{\varepsilon}_{k+q\downarrow} + \tilde{\varepsilon}_{k\downarrow}\right) \langle c_{k\downarrow}(t)c_{k+q\uparrow}(t) \rangle
\]
\[
= -\frac{U}{V} \sum_{k'} \langle c_{k'\uparrow}(t)c_{k'\downarrow}(t)\rangle \left[ f_{0}(\tilde{\varepsilon}_{k+q\downarrow}) - f_{0}(\tilde{\varepsilon}_{k\downarrow}) \right] \tag{29.8.29}
\]
\[
-\frac{1}{2} g_{e}\mu_{B} H_{\text{ext}}^{z}(q, t) \frac{1}{V} \left[ f_{0}(\tilde{\varepsilon}_{k+q\downarrow}) - f_{0}(\tilde{\varepsilon}_{k\downarrow}) \right].
\]

Dividing the temporal Fourier transform by the energy factor and summing over the momentum \(k\) gives

\[
\langle n_{\uparrow}(q, \omega) \rangle = \left[ \frac{1}{2} g_{e}\mu_{B} \mu_{0} H_{\text{ext}}^{z}(q, \omega) - U \langle n_{\uparrow}(q, \omega) \rangle \right]
\]
\[
\times \frac{1}{V} \sum_{k} \frac{f_{0}(\tilde{\varepsilon}_{k+q\uparrow}) - f_{0}(\tilde{\varepsilon}_{k\uparrow})}{\hbar\omega - \tilde{\varepsilon}_{k+q\uparrow} + \tilde{\varepsilon}_{k\uparrow}} \tag{29.8.30}
\]

and
\[ \langle n_1(q, \omega) \rangle = \left[ -\frac{i}{2} g_e \mu_B \mu_0 H_{ext}^z(q, \omega) - U \langle n_1(q, \omega) \rangle \right] \times \frac{1}{V} \sum_k \frac{f_0(\tilde{\varepsilon}_{k+q}) - f_0(\tilde{\varepsilon}_{k})}{\hbar \omega - \tilde{\varepsilon}_{k+q_1} + \tilde{\varepsilon}_{k_1}}. \]  

(29.8.31)

We introduce the notation

\[ \Sigma_{0\sigma}(q, \omega) = \frac{1}{V} \sum_k \frac{f_0(\tilde{\varepsilon}_{k+q_1}) - f_0(\tilde{\varepsilon}_{k})}{\hbar \omega - \tilde{\varepsilon}_{k+q_\sigma} + \tilde{\varepsilon}_{k_\sigma}}. \]  

(29.8.32)

The solution of (29.8.30) and (29.8.31) then takes the form

\[ \langle n_1(q, \omega) \rangle = \frac{1}{2} g_e \mu_B \mu_0 \Sigma_{0\uparrow}(q, \omega) \left[ 1 + U \Sigma_{0\downarrow}(q, \omega) \right] \frac{H_{ext}^z(q, \omega)}{1 - U^2 \Sigma_{0\uparrow}(q, \omega) \Sigma_{0\downarrow}(q, \omega)} \]  

(29.8.33)

\[ \langle n_1(q, \omega) \rangle = -\frac{1}{2} g_e \mu_B \mu_0 \Sigma_{0\downarrow}(q, \omega) \left[ 1 + U \Sigma_{0\uparrow}(q, \omega) \right] \frac{H_{ext}^z(q, \omega)}{1 - U^2 \Sigma_{0\uparrow}(q, \omega) \Sigma_{0\downarrow}(q, \omega)} \]  

(29.8.36)

\[ \langle n_1(q, \omega) \rangle = -\frac{1}{2} g_e \mu_B \mu_0 \Sigma_{0\downarrow}(q, \omega) \left[ 1 + U \Sigma_{0\uparrow}(q, \omega) \right] \frac{H_{ext}^z(q, \omega)}{1 - U^2 \Sigma_{0\uparrow}(q, \omega) \Sigma_{0\downarrow}(q, \omega)} \]  

(29.8.37)

To interpret this result we rewrite the interaction with the perturbing magnetic field in terms of \( n_\sigma(q) \):

\[ \mathcal{H}_1 = -\frac{1}{2} g_e \mu_B \mu_0 \frac{1}{V} \sum_q \frac{H_{ext}^z(q, t)}{\hbar \omega - \tilde{\varepsilon}_{k_1}} \left[ n_\uparrow(-q) - n_\downarrow(-q) \right] \]  

(29.8.38)

\[ \mathcal{H}_1 = -\frac{1}{2} g_e \mu_B \mu_0 \frac{1}{V} \sum_q \frac{H_{ext}^z(q, t)}{\hbar \omega - \tilde{\varepsilon}_{k_1}} \left[ n_\uparrow(-q) - n_\downarrow(-q) \right] \]  

Since the magnetization is proportional to the difference of \( n_1(q, \omega) \) and \( n_1(q, \omega) \), the parallel susceptibility consists of four terms:

\[ \chi_\parallel(q, \omega) = (\frac{1}{2} g_e \mu_B)^2 \mu_0 \left[ \Sigma_{1\uparrow}(q, \omega) - \Sigma_{1\downarrow}(q, \omega) - \Sigma_{\uparrow\downarrow}(q, \omega) + \Sigma_{\downarrow\uparrow}(q, \omega) \right], \]  

(29.8.39)

where

\[ \Sigma_{\sigma\sigma'}(q, \omega) = \frac{i}{\hbar} \int_0^\infty dt \int_0^\infty dt' \frac{1}{\hbar \omega - \tilde{\varepsilon}_{k_1}} \left[ n_\sigma(q, t), n_{\sigma'}(-q, t') \right]_-. \]  

(29.8.40)

These quantities are known already from the dielectric function. They are equal to the negative of the temporal Fourier transform of \( \Pi_{\sigma\sigma'}(q, t-t') \) defined in (29.1.33):

\[ \Sigma_{\sigma\sigma'}(q, \omega) = -\Pi_{\sigma\sigma'}(q, \omega). \]  

The \( \uparrow \) spin and \( \downarrow \) spin electrons contribute with equal weight to the density; therefore, the dielectric function contains the sum of the spin-resolved response
Electronic Response to External Perturbations

On the other hand, they appear in (29.8.36) with signs depending on the spin orientation. The RPA for the density–density response function could be visualized (see Fig. 29.5) as an infinite series of diagrams containing consecutive polarization bubbles. When a similar approximation is made for the susceptibility, we have to take into account that the dielectric function was calculated for the spin-independent Coulomb repulsion, while here we consider a Hubbard model in which only electrons of opposite spins interact. Therefore, when the spin-resolved response function is calculated in the RPA for the Hubbard model and the propagation of the electron–hole pair is visualized by diagrams, the subsequent bubbles have to have opposite spin orientations as shown pictorially in Fig. 29.14.

\[ \Sigma_{\uparrow\uparrow} = \begin{array}{c}
\text{Diagram 1} \\
\text{Diagram 2} \\
\text{Diagram 3} \\
\vdots
\end{array} \]

Fig. 29.14. The simplest processes contributing to the longitudinal susceptibility

Owing to this spin restriction, the sum of the bubble series gives

\[ \Sigma_{\uparrow\uparrow}(q, \omega) = \frac{\Sigma_{0\uparrow}(q, \omega)}{1 - U^2 \Sigma_{0\uparrow}(q, \omega) \Sigma_{0\downarrow}(q, \omega)} \]  \hspace{1cm} (29.8.39)

and

\[ \Sigma_{\uparrow\downarrow}(q, \omega) = \frac{-\Sigma_{0\uparrow}(q, \omega) U \Sigma_{0\downarrow}(q, \omega)}{1 - U^2 \Sigma_{0\uparrow}(q, \omega) \Sigma_{0\downarrow}(q, \omega)}. \]  \hspace{1cm} (29.8.40)

Summing up these expressions with the signs given in (29.8.36) we recover exactly the expression derived earlier for the longitudinal susceptibility. Thus the result of the equation-of-motion method is a straightforward extension of the renormalized RPA to the Hubbard model.

If the material is unpolarized, \( \Sigma_{0\uparrow} \) and \( \Sigma_{0\downarrow} \) are equal. Denoting their common value by \( \Sigma_0 \), we have

\[ \langle n_{\uparrow}(q, \omega) \rangle = -\langle n_{\downarrow}(q, \omega) \rangle = \frac{\frac{1}{2} g_0 \mu B \mu_0 \Sigma_0(q, \omega)}{1 - U \Sigma_0(q, \omega)} H_{ext}^z(q, \omega). \]  \hspace{1cm} (29.8.41)

Thus we get

\[ \langle m^z(q, \omega) \rangle = \frac{\frac{1}{2} g_0^2 \mu_B^2 \mu_0 \Sigma_0(q, \omega)}{1 - U \Sigma_0(q, \omega)} H_{ext}^z(q, \omega) \]  \hspace{1cm} (29.8.42)

for the \( z \)-component of the magnetic-moment density, and the longitudinal magnetic susceptibility becomes
\[
\chi_{\parallel}(q, \omega) = \frac{\frac{1}{2} g_e^2 \mu_B^2 \mu_0 \Sigma_0(q, \omega)}{1 - U \Sigma_0(q, \omega)}. \tag{29.8.43}
\]

When taking the limit \(\omega \to 0\) first and then \(q \to 0\), \(\Sigma_0(0, 0)\) is just the density of states for a single spin orientation. We then recover (29.8.11) derived for the static susceptibility. This expression can thus be considered as its generalization to the dynamical susceptibility.

Equation (29.8.43) for the susceptibility is formally very similar to the density–density response function (29.2.14) derived in the RPA. There is, however, an important difference. \(\Pi_0\) appearing in the denominator of (29.2.14) is equal to the negative of the density of states in the static, long-wavelength limit. This is due to the sign difference in (29.8.38). Thus, the Coulomb repulsion leads to a weakening of density fluctuations, but enhances magnetic fluctuations. Charge fluctuations can be enhanced by attractive interactions. Such an interaction can be mediated between electrons by long-wavelength acoustic phonons, as we have seen in Chapter 23, and the enhanced density fluctuations may give rise to the formation of static charge-density waves. This will be further discussed in Chapter 33.

29.8.3 Transverse Dynamical Susceptibility

In certain resonance experiments the weak high-frequency field \(H_{\text{ext}}\) is perpendicular to the homogeneous magnetic field \(H\). Choosing again the direction of the homogeneous field as the \(z\)-axis, it is convenient to use the linear combinations

\[
H_{\text{ext}}^\pm = H_{\text{ext}}^x \pm i H_{\text{ext}}^y
\]

for the perturbing field. The magnetic-moment density and the spin density will be expressed similarly by the linear combinations

\[
m^\pm = m^x \pm im^y, \quad s^\pm = s^x \pm is^y,
\]

instead of the \(x\)- and \(y\)-components of the \(m\) and \(s\) operators. The Hamiltonian describing the interaction with the perturbing field is then

\[
\mathcal{H}_1(t) = -\frac{1}{2} \mu_0 \frac{1}{V} \sum_q \left[ H_{\text{ext}}^+(q, t)m^-(q) + H_{\text{ext}}^-(q, t)m^+(q) \right] \tag{29.8.46}
\]

\[
= -\frac{1}{2} g_e \mu_B \mu_0 \frac{1}{V} \sum_q \left[ H_{\text{ext}}^+(q, t)s^-(q) + H_{\text{ext}}^-(q, t)s^+(q) \right]
\]

\[
= -\frac{1}{2} g_e \mu_B \mu_0 \frac{1}{V} \sum_{kq} \left[ H_{\text{ext}}^+(q, t)c_{k+q\uparrow}^c c_{k\downarrow} + H_{\text{ext}}^-(q, t)c_{k+q\downarrow}^c c_{k\uparrow} \right],
\]

where we used the second-quantized expressions

\[
s^+(q) = \sum_k c_{k\uparrow}^c c_{k+q\downarrow}, \quad s^-(q) = \sum_k c_{k\downarrow}^c c_{k+q\uparrow}.
\]

\[
\tag{29.8.47}
\]
The response to the transverse field can be characterized by the transverse susceptibility:

\[
\chi_{\perp}(q, \omega) = \frac{\langle m^{+}(q, \omega) \rangle}{H^{\perp}_{\text{ext}}(q, \omega)} = \frac{g_{e}\mu_{B}\langle s^{+}(q, \omega) \rangle}{H^{\perp}_{\text{ext}}(q, \omega)}. \tag{29.8.48}
\]

To calculate the expectation value \(\langle s^{+}(q, \omega) \rangle\) we use again the equation-of-motion method. Here the quantity \(\langle c^{\dagger}_{k\uparrow}(t)c_{k+q\downarrow}(t) \rangle\) has to be studied. The equations for the creation and annihilation operators are

\[
\left(-\frac{\hbar}{i}\frac{d}{dt} + \varepsilon_{k\uparrow}\right)c^{\dagger}_{k\uparrow}(t) = -\frac{U}{V} \sum_{k'q'} c^{\dagger}_{k+q'\downarrow}(t)c^{\dagger}_{k'q}(t)c_{k'q_1}(t) \tag{29.8.49}
\]

\[
+ \frac{1}{2} g_{e}\mu_{B}\mu_{0} \frac{1}{V} \sum_{q'} H^{\perp}_{\text{ext}}(q', t)c^{\dagger}_{k+q\perp}(t)
\]

and

\[
\left(-\frac{\hbar}{i}\frac{d}{dt} - \varepsilon_{k+q\downarrow}\right)c_{k+q\downarrow}(t) = \frac{U}{V} \sum_{k'q'} c_{k'q}(t)c_{k'q'}(t)c_{k+q-q'\downarrow}(t) \tag{29.8.50}
\]

\[
- \frac{1}{2} g_{e}\mu_{B}\mu_{0} \frac{1}{V} \sum_{q'} H^{\perp}_{\text{ext}}(q', t)c_{k+q-q'\downarrow}(t).
\]

When the three-operator terms are linearized (decoupled) by replacing the product of two operators by its expectation value, as was done in calculating the longitudinal susceptibility, these equations lead to

\[
\langle s^{+}(q, \omega) \rangle = \left[\frac{1}{2} g_{e}\mu_{B}\mu_{0}H^{\perp}_{\text{ext}}(q, \omega) + U\langle s^{+}(q, \omega) \rangle\right]\Sigma_{\perp}^{0}(q, \omega), \tag{29.8.51}
\]

where

\[
\Sigma_{\perp}^{0}(q, \omega) = \frac{1}{V} \sum_{k} \frac{f_{0}(\tilde{\varepsilon}_{k+q\uparrow}) - f_{0}(\tilde{\varepsilon}_{k\uparrow})}{\hbar\omega - \tilde{\varepsilon}_{k+q\downarrow} + \tilde{\varepsilon}_{k\downarrow}}. \tag{29.8.52}
\]

The solution of this equation yields

\[
\langle s^{+}(q, \omega) \rangle = \frac{\frac{1}{2} g_{e}\mu_{B}\mu_{0} \Sigma_{\perp}^{0}(q, \omega)}{1 - U \Sigma_{\perp}^{0}(q, \omega)} H^{\perp}_{\text{ext}}(q, \omega), \tag{29.8.53}
\]

from which we find

\[
\chi_{\perp}(q, \omega) = \frac{\frac{1}{2} g_{e}^{2}\mu_{B}^{2}\mu_{0}\Sigma_{\perp}^{0}(q, \omega)}{1 - U \Sigma_{\perp}^{0}(q, \omega)} \tag{29.8.54}
\]

for the transverse susceptibility. This quantity will be considered in Chapter 33 when spin-density fluctuations will be studied. Notice that this expression is identical to that obtained earlier for the longitudinal susceptibility when the system is unpolarized.
It is interesting to see which processes contribute to the transverse susceptibility in this approximation. For that we recall that according to linear response theory the transverse susceptibility is the temporal Fourier transform of the retarded response function

\[
\chi_\perp(q, t - t') = \frac{1}{2} \mu_0 \frac{i}{\hbar} \theta(t - t') \frac{1}{V} \left\langle \left[ m^+(q, t), m^-(-q, t') \right] \right\rangle.
\]  

(29.8.55)

When the spin density is used instead of the magnetic moment, we have

\[
\chi_\perp(q, \omega) = \frac{1}{2} g_\text{e}^2 \mu_0^2 \mu_0 \Sigma_\perp(q, \omega),
\]

(29.8.56)

where

\[
\Sigma_\perp(q, \omega) = \frac{i}{\hbar} \int_0^\infty dt' e^{i\omega(t-t')} \delta(t-t') \frac{1}{V} \left\langle \left[ s^+(q, t), s^-(-q, t') \right] \right\rangle.
\]

(29.8.57)

When \( s^+ \) and \( s^- \) are written in the second-quantized form, one sees that this response function describes the propagation of an electron–hole pair with opposite spins. The electron and the hole created at time \( t' \) interact with each other and with the other electrons of the Fermi sea before being annihilated at time \( t \). The susceptibility derived from the equation of motion is just the contribution of the processes shown diagrammatically in Fig. 29.15, when the series is continued up to infinity. Since the analytic contributions of these diagrams form a geometric progression, the summed-up form is easily obtained.

\[
\Sigma_\perp = \begin{array}{c}
\text{Fig. 29.15. The simplest processes taken into account in the transverse susceptibility}
\end{array}
\]

29.8.4 Ruderman–Kittel Oscillations

We know from Chapter 16 and from our earlier discussions in this chapter that a charged impurity distorts the electron states around itself. The external charge is fully screened in metals by the accumulated charge density. The spatial oscillations of this decaying charge density are called Friedel oscillations. Similar spatial oscillations may appear in the spin density of electrons when the impurity has a magnetic moment, as mentioned already in Chapter 14. We rederive here this oscillating spin density.

We saw in Chapter 24, in connection with the Kondo effect, that the interaction between conduction electrons and localized magnetic moments (spins)
of a magnetic impurity can be described by the so-called $s$–$d$ interaction. When a single localized moment is placed into the system at the origin and the quantization axis is in the $z$-direction, then

$$
\mathcal{H}_{s-d} = -J \hat{\psi}_{\alpha}^{\dagger}(0) \mathbf{S} \cdot \sigma_{\alpha\beta} \hat{\psi}_{\beta}(0)
$$

$$
= -\frac{J}{V} \sum_{kk'} \left[ S^+ c_{k'\uparrow}^\dagger c_{k\uparrow} + S^- c_{k'\downarrow}^\dagger c_{k\downarrow} + S^z \left( c_{k'\uparrow}^\dagger c_{k\uparrow}^\dagger - c_{k'\downarrow}^\dagger c_{k\downarrow} \right) \right].
$$

(29.8.58)

Let us assume that the system of electrons is in thermal equilibrium, the charge and spin densities are homogeneous, and the localized spin is originally in state $|M\rangle$ for which $S^z |M\rangle = M |M\rangle$. We are interested in the modification of the electronic wavefunction and the spatial distribution of the spin density around the localized spin. Technically it is easier to determine this spatial variation of the spin density than to derive the Friedel oscillations in the charge density since the interaction with the magnetic impurities is short ranged, while the Coulomb interaction is long ranged.

The wavefunction of the perturbed electron system can be written in Slater-determinant form, where the single-particle states are perturbed plane waves obtained by taking the interaction with the localized spin into account. If the electron has wave vector $k$ and spin $\uparrow$, and the localized spin is in state $|M\rangle$, the unperturbed state is

$$
|k\uparrow, M\rangle = c_{k\uparrow}|0\rangle |M\rangle ,
$$

(29.8.59)

where $|0\rangle$ denotes the vacuum of electrons. This state will be mixed by the $s$–$d$ interaction to states $|k'\sigma', M'\rangle$ in which both the wave vector and the spin of the electron as well as the orientation of the impurity spin can differ from that in the initial state. In first order of perturbation theory, the perturbed wavefunction is

$$
|k\uparrow, M\rangle^{(1)} = |k\uparrow, M\rangle + \sum_{k'\sigma'} |k'\sigma', M'\rangle \frac{\langle k'\sigma', M' | \mathcal{H}_{s-d} | k\uparrow, M \rangle}{\varepsilon_k - \varepsilon_{k'}}.
$$

(29.8.60)

There is no summation over $M'$; it cannot be chosen arbitrarily, because the $z$-component of the total spin is conserved. Taking the matrix elements of the interaction Hamiltonian we find

$$
|k\uparrow, M\rangle^{(1)} = |k\uparrow, M\rangle - \frac{1}{V} \sum_{k'} \frac{J}{\varepsilon_k - \varepsilon_{k'}} \left[ \langle M + 1 | S^+ | k'\downarrow, M + 1 \rangle + \langle M | S^z | k'\uparrow, M \rangle \right].
$$

(29.8.61)

Similarly

$$
|k\downarrow, M\rangle^{(1)} = |k\downarrow, M\rangle - \frac{1}{V} \sum_{k'} \frac{J}{\varepsilon_k - \varepsilon_{k'}} \left[ \langle M - 1 | S^- | k'\uparrow, M - 1 \rangle - \langle M | S^z | k'\downarrow, M \rangle \right].
$$

(29.8.62)
In an isotropic system, where the unperturbed states are plane waves, we obtain

\[ |k \uparrow, M \rangle^{(1)} = \frac{1}{\sqrt{V}} e^{i k \cdot r} |\uparrow, M \rangle - J V^{3/2} \sum_{k'} \frac{e^{i k' \cdot r}}{\varepsilon_k - \varepsilon_{k'}} \times [ \langle M + 1 | S^+ | M \rangle \downarrow, M + 1 + \langle M | S^z | M \rangle \uparrow, M ] \]

(29.8.63)

and

\[ |k \downarrow, M \rangle^{(1)} = \frac{1}{\sqrt{V}} e^{i k \cdot r} |\downarrow, M \rangle - J V^{3/2} \sum_{k'} \frac{e^{i k' \cdot r}}{\varepsilon_k - \varepsilon_{k'}} \times [ \langle M - 1 | S^- | M \rangle \uparrow, M - 1 - \langle M | S^z | M \rangle \downarrow, M ] . \]

(29.8.64)

The integration over \( k' \) can be done using (C.1.66) yielding

\[ |k \uparrow, M \rangle^{(1)} = \frac{1}{\sqrt{V}} e^{i k \cdot r} |\uparrow, M \rangle - \frac{1}{\sqrt{V}} m_e J \cos kr \frac{\cos \theta}{2 \pi r \hbar^2} \times \left( \sqrt{S(S+1) - M(M+1)} \downarrow, M + 1 + M \uparrow, M \right) \]

(29.8.65)

and

\[ |k \downarrow, M \rangle^{(1)} = \frac{1}{\sqrt{V}} e^{i k \cdot r} |\downarrow, M \rangle - \frac{1}{\sqrt{V}} m_e J \cos kr \frac{\cos \theta}{2 \pi r \hbar^2} \times \left( \sqrt{S(S+1) - M(M-1)} \uparrow, M - 1 - M \downarrow, M \right) . \]

(29.8.66)

The density due to electrons occupying these states is obtained by calculating the quantities \((M, k \uparrow | k \uparrow, M \rangle^{(1)})\) and \((M, k \downarrow | k \downarrow, M \rangle^{(1)})\). We find

\[ n_\uparrow(k, r) = \frac{1}{V} \left[ 1 - \frac{m_e J \cos kr}{\pi r \hbar^2} M \cos(k \cdot r) \right] , \]

(29.8.67)

\[ n_\downarrow(k, r) = \frac{1}{V} \left[ 1 + \frac{m_e J \cos kr}{\pi r \hbar^2} M \cos(k \cdot r) \right] . \]

(29.8.68)

The total density of the up- and down-spin electrons is obtained by summing the contribution of all occupied states. At temperature \( T = 0 \), this is equivalent to integrating over all \( k \) vectors inside the Fermi sphere. This gives

\[ n_\uparrow(r) = \frac{k_F^3}{6\pi^2} \left[ 1 + \frac{6m_e J M k_F}{\pi r \hbar^2} g(2k_F r) \right] , \]

(29.8.69)

\[ n_\downarrow(r) = \frac{k_F^3}{6\pi^2} \left[ 1 - \frac{6m_e J M k_F}{\pi r \hbar^2} g(2k_F r) \right] . \]

(29.8.70)

where \( g(x) \) is the decaying oscillatory function given in (29.3.24).
This shows that the localized moment perturbs the spatial distribution of conduction electrons in such a way that the number density $n(r) = n_\uparrow(r) + n_\downarrow(r)$, and hence the charge density, remains uniform, but a spatially varying spin density $\sigma(r) = n_\uparrow(r) - n_\downarrow(r)$ appears in the originally unpolarized system. This spin density oscillates in space and decays with the third power of the distance from the impurity. These oscillations are known as the Ruderman–Kittel oscillations. The periodicity of the oscillations, their wavelength $\lambda$, is determined by the relation $2k_F\lambda = 2\pi$. As has been mentioned already and derived in Appendix I, this oscillating-induced spin density gives rise to the spatially oscillating RKKY interaction between magnetic moments placed at a distance $r$ in a metal.

The results derived above are modified at finite temperatures for two reasons. On the one hand, the Fermi distribution function is smeared out over an interval of width $k_BT$ around the Fermi energy, and this leads to a factor $\exp(-\pi k_F r k_B T / \varepsilon_F)$ in the charge distribution. On the other hand, an extra factor $\exp(-r/l)$ may appear due to the finite mean free path $l$ of electrons.

This oscillating spin density around a magnetic impurity can be observed experimentally, e.g., in the shift of the resonance frequency of nuclear magnetic resonance.

**Further Reading**

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