
Transport Phenomena

In Chapter 16 we already discussed the propagation of electric and heat currents in the simplest model of metals, the classical Drude model, and then in the quantum mechanical Sommerfeld model, however the treatment was not consistently quantum mechanical in the latter. Since the complete solution of the quantum mechanical problem of electrons in an applied electric field or under other external forces (for example, a temperature gradient) is not known, we tacitly opted for the application of the semiclassical treatment by assuming that the occupation of the electron states can be characterized by a position- and wave-vector-dependent nonequilibrium stationary distribution function $f(\mathbf{r}, \mathbf{k})$. Having given a more precise meaning to the semiclassical approximation in Chapter 21, we are now in the position to apply it to the description of conduction phenomena, and examine the current carried by the electrons moving in the periodic potential of the lattice.

In addition to the semiclassical approximation, our previous considerations were also based on the assumption that, just like in the Drude model, the effects of collisions can be taken into account by a relaxation time in the Sommerfeld model, too. Since this quantity is introduced phenomenologically, nothing can be said about its temperature dependence within these models – and consequently, the correct results for the temperature dependence of the electrical resistivity and thermal conductivity cannot be derived, either.

Moreover, these models may, at best, be applied to the description of the properties of simple metals, in which the conduction electrons behave like free electrons; the transport properties of semiconductors or transition metals with a narrow d -band are obviously outside their realm. Therefore another approach is required for the description of the transport properties of Bloch electrons and phonons interacting with them.

Before starting the discussion of the characteristic phenomena in solids, we briefly summarize the most important results of the irreversible thermodynamical treatment of transport phenomena. Then we introduce the Boltzmann equation, whose solution gives the nonequilibrium distribution of electrons and phonons in the presence of an external perturbation. To determine

the distribution function, we shall first study the Boltzmann equation in the relaxation-time approximation, and then take into account the scattering of electrons more accurately than before. Finally, we shall use the results to calculate the temperature dependence of the electrical resistivity and thermal conductivity of metals and semiconductors.

24.1 General Formulation of Transport Phenomena

In a system of charged particles an applied electric field induces an electric current, while a temperature gradient generates a heat current. However, the heat current may also be carried by uncharged particles, for example, phonons. The behavior of solids is primarily determined by the propagation of these currents inside them. In multicomponent materials the particle currents of individual components are also studied, while in semiconductors the currents carried by electrons and holes are customarily separated.

By writing the electric field as the gradient of an electrostatic potential, currents are seen to be induced by the gradient of this potential and the temperature gradient. The diffusion current of particles appears when the concentration has a nonvanishing gradient. In general, such gradients are the driving forces of currents.

In solids the electric field is usually sufficiently weak to justify dealing with linear phenomena alone. Then Ohm's law implies

$$\mathbf{j} = \boldsymbol{\sigma} \mathbf{E} = -\boldsymbol{\sigma} \nabla \varphi, \quad (24.1.1)$$

where $\boldsymbol{\sigma}$ is the conductivity tensor. For a temperature gradient, too, the response to the perturbation – the heat current – is proportional to the driving force (unless its spatial variations are excessively rapid):

$$\mathbf{j}_Q = -\lambda \nabla T, \quad (24.1.2)$$

where λ is the thermal or heat conductivity. If the particle density n is not uniform, diffusion leads to a nonvanishing particle-current density:

$$\mathbf{j}_n = -D \nabla n, \quad (24.1.3)$$

where D is the diffusion coefficient.

It is well known from classical physics that an electric field can also induce a heat current, and a temperature gradient can generate an electric current. Likewise, electric and heat currents are induced when the chemical potential shows spatial variations. The corresponding component of the current is proportional to the gradient of the chemical potential. It was demonstrated in Chapter 16 that the coefficients of these cross effects are related to each other in a simple way. We shall give a more general formulation of this statement below.

24.1.1 Currents and Driving Forces

In the analysis of currents, we need to distinguish particle currents, electric currents, energy currents, heat currents, and entropy currents. Their densities are denoted by \mathbf{j}_n , \mathbf{j} , \mathbf{j}_E , \mathbf{j}_Q , and \mathbf{j}_S , respectively. The relationships between \mathbf{j}_n and \mathbf{j} , and \mathbf{j}_Q and \mathbf{j}_S are easily established:

$$\mathbf{j}_Q = T\mathbf{j}_S \quad (24.1.4)$$

is generally valid, while for the density of the electric current carried by electrons

$$\mathbf{j} = -e\mathbf{j}_n. \quad (24.1.5)$$

One more relation can be written down if changes in the volume can be neglected ($dV = 0$), which is a fairly good approximation for solids. From the thermodynamic relation

$$TdS = dE - \mu dN \quad (24.1.6)$$

we then have

$$T\mathbf{j}_S = \mathbf{j}_E - \mu\mathbf{j}_n. \quad (24.1.7)$$

The same thermodynamic relation also implies a formula between the time rates of change of the entropy, energy, and particle number:

$$T\frac{\partial S}{\partial t} = \frac{\partial E}{\partial t} - \mu\frac{\partial N}{\partial t}. \quad (24.1.8)$$

When each quantity is referred to unit volume, and therefore denoted by the corresponding lowercase letter (except for the energy density, which is denoted by w to distinguish it from the elementary charge e), we have

$$T\frac{\partial s}{\partial t} = \frac{\partial w}{\partial t} - \mu\frac{\partial n}{\partial t}. \quad (24.1.9)$$

The particle density and the particle-current density have to satisfy the continuity equation

$$\frac{\partial n}{\partial t} + \operatorname{div} \mathbf{j}_n = 0. \quad (24.1.10)$$

A similar equation is valid for the energy density and energy-current density; however, the generation of Joule heat is taken into account by an additional term in the energy balance:

$$\frac{\partial w}{\partial t} + \operatorname{div} \mathbf{j}_E = \mathbf{E} \cdot \mathbf{j}. \quad (24.1.11)$$

The analogous equation for the entropy density also contains an additional term on the right-hand side that corresponds to the local entropy production:

$$\frac{\partial s}{\partial t} + \operatorname{div} \mathbf{j}_S = \dot{s}. \quad (24.1.12)$$

Using the previous equations, \dot{s} can be written as

$$\begin{aligned}\dot{s} &= \frac{1}{T} \left(\frac{\partial w}{\partial t} - \mu \frac{\partial n}{\partial t} \right) + \operatorname{div} \frac{\mathbf{j}_Q}{T} \\ &= \frac{1}{T} \left(\mathbf{E} \cdot \mathbf{j} - \operatorname{div} \mathbf{j}_E + \mu \operatorname{div} \mathbf{j}_n + \operatorname{div} \mathbf{j}_Q - \mathbf{j}_Q \cdot \frac{\nabla T}{T} \right).\end{aligned}\quad (24.1.13)$$

From (24.1.4) and (24.1.7) we have

$$\operatorname{div} \mathbf{j}_Q = \operatorname{div} \mathbf{j}_E - \mathbf{j}_n \cdot \nabla \mu - \mu \operatorname{div} \mathbf{j}_n, \quad (24.1.14)$$

and so the entropy-production formula can be simplified to

$$\begin{aligned}\dot{s} &= \frac{1}{T} \left\{ \mathbf{E} \cdot \mathbf{j} - \mathbf{j}_n \cdot \nabla \mu - \mathbf{j}_Q \cdot \frac{\nabla T}{T} \right\} \\ &= \frac{1}{T} \left\{ \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) \cdot \mathbf{j} - \frac{\nabla T}{T} \cdot \mathbf{j}_Q \right\}.\end{aligned}\quad (24.1.15)$$

Rewriting this as

$$\dot{s} = \frac{1}{T} (\mathbf{X}_e \cdot \mathbf{j} + \mathbf{X}_Q \cdot \mathbf{j}_Q), \quad (24.1.16)$$

the multiplying factor of the current densities is called the driving force of the current. If, in addition to the electric and heat currents, other currents also flow in the system, the corresponding driving force is defined through the relation

$$\dot{s} = \frac{1}{T} \sum_i \mathbf{X}_i \cdot \mathbf{j}_i. \quad (24.1.17)$$

The previous formulas confirm that the driving force of the electric current is not simply the electric field \mathbf{E} but the combination $\mathbf{E} + \nabla \mu/e$. When the electric field is derived from a scalar potential,

$$\mathbf{X}_e = \mathbf{E} + \frac{\nabla \mu}{e} = -\nabla \left(\varphi - \frac{\mu}{e} \right), \quad (24.1.18)$$

that is, the driving force is not the gradient of the electrostatic potential φ but that of the electrochemical potential $\varphi - \mu/e$, as was demonstrated for free electrons on page 53. Similarly, the driving force of the heat current is not simply $-\nabla T$ but

$$\mathbf{X}_Q = -\frac{\nabla T}{T}. \quad (24.1.19)$$

24.1.2 Onsager Relations

As mentioned earlier, in the overwhelming majority of transport phenomena in solids the currents can be taken to be proportional to the driving forces:

$$\mathbf{j}_i = \sum_j L_{ij} \mathbf{X}_j. \quad (24.1.20)$$

According to irreversible thermodynamics, the cross effects satisfy the Onsager relations in this linear approximation:

$$L_{ij}^{\alpha\beta} = L_{ji}^{\beta\alpha}, \quad (24.1.21)$$

while in a magnetic field

$$L_{ij}^{\alpha\beta}(B) = L_{ji}^{\beta\alpha}(-B). \quad (24.1.22)$$

When only an electric field and a temperature gradient are applied, and only the electric and heat currents are considered,

$$\begin{aligned} \mathbf{j} &= L_{11} \left(\mathbf{E} + \frac{\nabla\mu}{e} \right) + L_{12} \left(-\frac{\nabla T}{T} \right), \\ \mathbf{j}_Q &= L_{21} \left(\mathbf{E} + \frac{\nabla\mu}{e} \right) + L_{22} \left(-\frac{\nabla T}{T} \right). \end{aligned} \quad (24.1.23)$$

In the Sommerfeld model these coefficients are scalars on account of the isotropy of the electron gas. Comparison with (16.3.32) shows that L_{12} and L_{21} are equal, and their value is the negative of the integral K_1 defined in (16.3.33). The equality of L_{12} and L_{21} is now seen not to be accidental but the consequence of the Onsager relations of nonequilibrium thermodynamics, and is thus generally valid.

24.2 Boltzmann Equation

An exact quantum mechanical treatment of conduction phenomena requires the apparatus of the many-body problem. As we shall briefly discuss in Chapter 36, this is indeed necessary in disordered systems. However, in solid-state physics we usually deal with systems in which the mean free path of electrons is much larger than their de Broglie wavelength, and therefore the conduction electrons can be considered to make up a semiclassical electron gas as far as the conduction properties are concerned – so their equation of motion is known. The kinetic theory of gases can then be applied to this electron gas, with the difference that the most important collision mechanism is not the scattering of particles by one another but the interaction with the crystal lattice, its vibrations or defects. The reason why transport phenomena were not analyzed in depth in Chapter 16 on the Sommerfeld model is that the reader may not have been familiar with the details of the interaction between the electrons and the vibrating lattice (the electron–phonon interaction).

In thermal equilibrium the occupation of electron states is characterized by the Fermi–Dirac distribution, while phonon states are described by the Bose–Einstein distribution. In the semiclassical approximation the nonequilibrium

state can be specified by a nonequilibrium distribution function. We shall first derive the Boltzmann equation that determines this distribution function, and then present the approximations used for solving it.

24.2.1 Nonequilibrium Distribution Function

Consider a point \mathbf{r}, \mathbf{k} in the phase space of the position and wave vector of electrons, and denote the number of electrons that are inside the phase-space volume element $d\mathbf{r} d\mathbf{k}$ around the point \mathbf{r}, \mathbf{k} at time t by $dN(\mathbf{r}, \mathbf{k}, t)$. The nonequilibrium distribution function $f(\mathbf{r}, \mathbf{k}, t)$ is then defined as

$$dN(\mathbf{r}, \mathbf{k}, t) = f(\mathbf{r}, \mathbf{k}, t) \frac{d\mathbf{r} d\mathbf{k}}{4\pi^3}. \quad (24.2.1)$$

This formula contains the information that the \mathbf{k} -space density of the allowed wave vectors is $V/(2\pi)^3$ in a sample of volume V , and the factor 2 due to the two possible spin orientations is also included. The electric current density at point \mathbf{r} at time t is then

$$\mathbf{j}(\mathbf{r}, t) = -e \int \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}_{\mathbf{k}} f(\mathbf{r}, \mathbf{k}, t), \quad (24.2.2)$$

while the heat-current density is

$$\mathbf{j}_Q(\mathbf{r}, t) = \int \frac{d\mathbf{k}}{4\pi^3} (\varepsilon_{\mathbf{k}} - \mu) \mathbf{v}_{\mathbf{k}} f(\mathbf{r}, \mathbf{k}, t). \quad (24.2.3)$$

If electrons populate several bands, then the number of electrons can be considered separately for each band. When dN_n of the dN electrons in the phase-space volume element occupy states of the band of index n , the distribution function for that band is defined by

$$dN_n(\mathbf{r}, \mathbf{k}, t) = f_n(\mathbf{r}, \mathbf{k}, t) \frac{d\mathbf{r} d\mathbf{k}}{4\pi^3}. \quad (24.2.4)$$

Since electrons in completely filled bands do not carry a net current, we shall be concerned with the contribution of incomplete shells in our treatment of transport phenomena. In most of our calculations we shall assume that there is a single band of interest, and thus suppress the band index. As individual bands contribute additively to the currents, the generalization to the case of multiple partially filled bands is straightforward.

In magnetic systems, the number of electrons in the volume element $d\mathbf{r} d\mathbf{k}$ may be different for the two spin orientations ($\sigma = \uparrow, \downarrow$). We shall also see examples where the strength of the interaction that governs the scattering of electrons depends on the orientation of the electron spin. Their proper treatment requires the introduction of a spin-dependent distribution function, which can be defined in terms of the number of spin- σ particles as

$$dN_\sigma(\mathbf{r}, \mathbf{k}, t) = f_\sigma(\mathbf{r}, \mathbf{k}, t) \frac{d\mathbf{r} d\mathbf{k}}{8\pi^3}. \quad (24.2.5)$$

Below we shall suppress the spin index, unless it is expressly needed.

In thermal equilibrium the distribution of the electrons is specified by the well-known Fermi function

$$f_0(\mathbf{k}) = \frac{1}{\exp[(\varepsilon_{\mathbf{k}} - \mu)/k_B T] + 1}. \quad (24.2.6)$$

If the temperature or the chemical potential is nonuniform, the distribution function contains their local values:

$$f_0(\mathbf{r}, \mathbf{k}) = \frac{1}{\exp[(\varepsilon_{\mathbf{k}} - \mu(\mathbf{r}))/k_B T(\mathbf{r})] + 1}. \quad (24.2.7)$$

Phonons are treated on the same footing. A temperature gradient modifies the phonon distribution with respect to the thermal equilibrium. Denoting the number of phonons of polarization λ in the region $d\mathbf{r} d\mathbf{q}$ around the point \mathbf{r}, \mathbf{q} of the phase space by dN_λ , the phonon distribution function $g_\lambda(\mathbf{r}, \mathbf{q}, t)$ is defined as

$$dN_\lambda(\mathbf{r}, \mathbf{q}, t) = g_\lambda(\mathbf{r}, \mathbf{q}, t) \frac{d\mathbf{r} d\mathbf{q}}{8\pi^3}. \quad (24.2.8)$$

Since phonons obey the Bose–Einstein statistics, and their chemical potential vanishes in thermal equilibrium, we have

$$g_\lambda^0(\mathbf{q}) = \frac{1}{\exp[\hbar\omega_\lambda(\mathbf{q})/k_B T] - 1}, \quad (24.2.9)$$

while if the system is in local equilibrium in a nonuniform temperature distribution,

$$g_\lambda^0(\mathbf{r}, \mathbf{q}) = \frac{1}{\exp[\hbar\omega_\lambda(\mathbf{q})/k_B T(\mathbf{r})] - 1}. \quad (24.2.10)$$

24.2.2 Boltzmann Equation for Electrons

To determine the nonequilibrium distribution function, the phase-space motion of the particles inside the volume element $d\mathbf{r} d\mathbf{k}$ around the point \mathbf{r}, \mathbf{k} at time t needs to be studied. If no collisions occur, then dt time later they are in the region $d\mathbf{r}' d\mathbf{k}'$ around \mathbf{r}', \mathbf{k}' , where the primed and unprimed quantities are related by $\mathbf{r}' = \mathbf{r} + \dot{\mathbf{r}} dt$ and $\mathbf{k}' = \mathbf{k} + \dot{\mathbf{k}} dt$. Because of the conservation of the particle number,

$$f(\mathbf{r}, \mathbf{k}, t) d\mathbf{r} d\mathbf{k} = f(\mathbf{r} + \dot{\mathbf{r}} dt, \mathbf{k} + \dot{\mathbf{k}} dt, t + dt) d\mathbf{r}' d\mathbf{k}'. \quad (24.2.11)$$

According to Liouville's theorem, the phase-space volume remains constant during the motion, $d\mathbf{r} d\mathbf{k} = d\mathbf{r}' d\mathbf{k}'$, and so

$$f(\mathbf{r} + \dot{\mathbf{r}} dt, \mathbf{k} + \dot{\mathbf{k}} dt, t + dt) = f(\mathbf{r}, \mathbf{k}, t). \quad (24.2.12)$$

For small time differences the linear-order expansion of the left-hand side gives

$$\frac{df}{dt} \equiv \frac{\partial f}{\partial t} + \dot{\mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = 0, \quad (24.2.13)$$

which is in fact the equation of continuity in phase space.

On the other hand, when collisions occur during the infinitesimal time interval dt , by which certain particles are scattered out of the phase-space trajectory (outscattering) – or other particles are scattered into the vicinity of the phase-space point \mathbf{r}', \mathbf{k}' (inscattering) – then a collision term appears on the right-hand side:

$$f(\mathbf{r} + \dot{\mathbf{r}} dt, \mathbf{k} + \dot{\mathbf{k}} dt, t + dt) = f(\mathbf{r}, \mathbf{k}, t) + \left(\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t} \right)_{\text{coll}} dt, \quad (24.2.14)$$

where

$$\left(\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t} \right)_{\text{coll}} dt = \left(\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t} \right)_{\text{in}} dt - \left(\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t} \right)_{\text{out}} dt \quad (24.2.15)$$

is the change in particle number due to the difference of inscattering and outscattering. Expanding this formula to linear order in dt ,

$$\frac{\partial f}{\partial t} + \dot{\mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}. \quad (24.2.16)$$

This is the *Boltzmann equation*.¹

In the semiclassical approximation the phase-space motion of electrons is given by the equations

$$\dot{\mathbf{r}} = \mathbf{v}_{\mathbf{k}} = \frac{1}{\hbar} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}}, \quad \hbar \dot{\mathbf{k}} = -e(\mathbf{E} + \mathbf{v}_{\mathbf{k}} \times \mathbf{B}). \quad (24.2.17)$$

Thus in the stationary case the distribution function can be determined by solving

$$\mathbf{v}_{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{r}} - \frac{e}{\hbar} (\mathbf{E} + \mathbf{v}_{\mathbf{k}} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{k}} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}. \quad (24.2.18)$$

Assuming that the distribution function is just slightly different from the thermal-equilibrium function f_0 , using the notation $f = f_0 + f_1$ we may transform the Boltzmann equation into an equation for the departure f_1 from the equilibrium distribution:

$$\begin{aligned} \mathbf{v}_{\mathbf{k}} \cdot \frac{\partial f_0}{\partial \mathbf{r}} - \frac{e}{\hbar} (\mathbf{E} + \mathbf{v}_{\mathbf{k}} \times \mathbf{B}) \cdot \frac{\partial f_0}{\partial \mathbf{k}} \\ = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} - \mathbf{v}_{\mathbf{k}} \cdot \frac{\partial f_1}{\partial \mathbf{r}} + \frac{e}{\hbar} (\mathbf{E} + \mathbf{v}_{\mathbf{k}} \times \mathbf{B}) \cdot \frac{\partial f_1}{\partial \mathbf{k}}. \end{aligned} \quad (24.2.19)$$

¹ L. BOLTZMANN, 1872.

Since f_0 depends on the wave and position vectors only through the combination $(\varepsilon_{\mathbf{k}} - \mu(\mathbf{r}))/k_{\text{B}}T(\mathbf{r})$, the left-hand side can be rewritten as

$$\begin{aligned} \mathbf{v}_{\mathbf{k}} \cdot \frac{\partial f_0}{\partial \mathbf{r}} - \frac{e}{\hbar} (\mathbf{E} + \mathbf{v}_{\mathbf{k}} \times \mathbf{B}) \cdot \frac{\partial f_0}{\partial \mathbf{k}} \\ = - \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \mathbf{v}_{\mathbf{k}} \cdot \left[-e \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) - \frac{\varepsilon_{\mathbf{k}} - \mu}{T} \nabla T \right]. \end{aligned} \quad (24.2.20)$$

The explicit magnetic-field dependence of the left-hand side has thus been eliminated. Nonetheless an implicit dependence remains, as the trajectory of electrons – and, consequently, their velocity, too – still depends on the applied field. This clearly shows the special role of the magnetic field: when the motion of electrons is examined, it cannot be considered as a weak perturbation to which electrons react linearly. The situation is different for the electric field. Customarily, only the linear response to the electric field is studied. As f_1 itself is proportional to the applied field, the term that is proportional to \mathbf{E} can be neglected on the right-hand side of (24.2.19), as it would lead to a quadratic correction. The Boltzmann equation for electrons is therefore

$$\begin{aligned} - \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \mathbf{v}_{\mathbf{k}} \cdot \left[-e \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) - \frac{\varepsilon_{\mathbf{k}} - \mu}{T} \nabla T \right] \\ = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} - \mathbf{v}_{\mathbf{k}} \cdot \frac{\partial f_1}{\partial \mathbf{r}} + \frac{e}{\hbar} (\mathbf{v}_{\mathbf{k}} \times \mathbf{B}) \cdot \frac{\partial f_1}{\partial \mathbf{k}}. \end{aligned} \quad (24.2.21)$$

We shall usually study conduction phenomena in uniform fields and in the presence of a constant temperature gradient, and be concerned with the dependence of the distribution function only on the wave vector and energy.

Up to now nothing has been said about how the collision term in the Boltzmann equation should be chosen. Therefore we shall first determine the collision term due to the scattering of electrons by the defects of a rigid lattice, and then turn to the collision terms in a vibrating lattice due to the electron–phonon interaction (coupled system of electrons and phonons). We shall also see what collision terms arise when phonons interact only among themselves.

24.2.3 Collision Term for Scattering by Lattice Defects

In a rigid lattice, the collision term comes from the interaction of electrons with other electrons and their scattering by lattice defects. The collision integral can be written down simply for the latter provided the matrix elements of the scattering by lattice defects are known.

Let us denote the probability for an electron in state \mathbf{k} to be scattered in time dt into an empty state in the volume element $d\mathbf{k}'$ around \mathbf{k}' by $W_{\mathbf{k}\mathbf{k}'} \frac{d\mathbf{k}'}{(2\pi)^3}$. Since the probability for a given state to be empty is $1 - f(\mathbf{k}')$, and the state \mathbf{k} is present with a weight $f(\mathbf{k})$, the probability of outscattering is

$$\left(\frac{\partial f}{\partial t}\right)_{\text{out}} = f(\mathbf{k}) \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}\mathbf{k}'} [1 - f(\mathbf{k}')] . \quad (24.2.22)$$

In the inscattering process electrons are scattered from \mathbf{k}' to \mathbf{k} ; this requires that \mathbf{k}' be occupied and \mathbf{k} empty initially. The probability of this process is therefore

$$\left(\frac{\partial f}{\partial t}\right)_{\text{in}} = [1 - f(\mathbf{k})] \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}'\mathbf{k}} f(\mathbf{k}') . \quad (24.2.23)$$

Since the spin is conserved in the scattering, there is no summation over the spin variable. The full collision integral of the two processes is

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \int \frac{d\mathbf{k}'}{(2\pi)^3} \{ W_{\mathbf{k}'\mathbf{k}} f(\mathbf{k}') [1 - f(\mathbf{k})] - W_{\mathbf{k}\mathbf{k}'} f(\mathbf{k}) [1 - f(\mathbf{k}')] \} . \quad (24.2.24)$$

When this is substituted into the Boltzmann equation, a nonlinear integrodifferential equation is obtained for the electronic distribution function even in the simplest case. Its solution obviously requires further approximations. Before turning to their discussion, let us write down the Boltzmann equation for the nonequilibrium distribution of phonons, which sometimes also play an important role in the determination of transport properties of solids.

24.2.4 Boltzmann Equation for Phonons

When the perturbations vary slowly both in space and time, the properties determined by the lattice vibrations (phonons) can also be treated in the semiclassical approximation – that is, a position- and time-dependent semiclassical distribution function can be introduced for phonons much in the same way as was done for electrons. Apart from piezoelectric effects, the electromagnetic field does not act on phonons; however, when a temperature gradient is present, the equilibrium distribution of phonons is disturbed, and they can also carry a heat current. Consequently, the equation governing the phase-space variations of the distribution function $g_\lambda(\mathbf{r}, \mathbf{q}, t)$ for phonons of polarization λ differs formally from the Boltzmann equation for electrons in the absence of the term arising from the variation of the wave vector:

$$\frac{\partial g_\lambda(\mathbf{r}, \mathbf{q}, t)}{\partial t} + \mathbf{c}_\lambda(\mathbf{q}) \cdot \frac{\partial g_\lambda(\mathbf{r}, \mathbf{q}, t)}{\partial \mathbf{r}} = \left(\frac{\partial g_\lambda}{\partial t}\right)_{\text{coll}} , \quad (24.2.25)$$

where $\mathbf{c}_\lambda(\mathbf{q})$ is the group velocity of phonons of polarization λ , which can be derived from the dispersion relation as

$$\mathbf{c}_\lambda(\mathbf{q}) = \frac{\partial \omega_\lambda(\mathbf{q})}{\partial \mathbf{q}} . \quad (24.2.26)$$

In the stationary case

$$c_\lambda \cdot \frac{\partial g_\lambda(\mathbf{r}, \mathbf{q}, t)}{\partial \mathbf{r}} = \left(\frac{\partial g_\lambda}{\partial t} \right)_{\text{coll}}. \quad (24.2.27)$$

By relating the spatial variations to the temperature gradient,

$$c_\lambda \cdot \nabla T \frac{\partial g_\lambda(\mathbf{r}, \mathbf{q}, t)}{\partial T} = \left(\frac{\partial g_\lambda}{\partial t} \right)_{\text{coll}}. \quad (24.2.28)$$

When the system of phonons is studied in itself, the decay and merger processes of phonons due to anharmonicity need to be taken into account to determine the collision integral. For simplicity, we shall consider only three-phonon processes, and neglect umklapp processes. The processes in which a phonon of wave vector \mathbf{q} can participate are shown in Fig. 24.1.

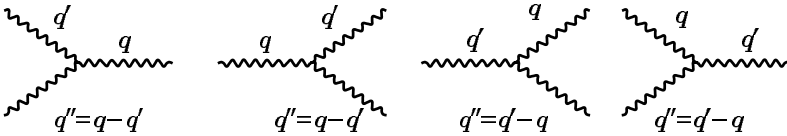


Fig. 24.1. Decay and merger processes with three phonons involved, which modify the distribution function of the phonons of wave vector \mathbf{q}

We shall denote by $W_{\mathbf{q}\mathbf{q}'}$ the transition probability of the process in which a phonon of wave vector \mathbf{q} decays into two phonons, \mathbf{q}' and $\mathbf{q}'' = \mathbf{q} - \mathbf{q}'$. Obviously, the inverse process – in which two phonons, \mathbf{q}' and $\mathbf{q}'' = \mathbf{q} - \mathbf{q}'$, merge into one, of wave vector \mathbf{q} – has the same transition probability. The number of phonons of wave vector \mathbf{q} is reduced by the first and increased by the second process, so they contribute to outscattering and inscattering, respectively. To determine the actual contribution, one has to sum over the possible values of \mathbf{q}' . It must, however, be borne in mind that for inscattering processes the transition probability $W_{\mathbf{q}\mathbf{q}'}$ has to be multiplied by the probability that the system initially contains the two phonons, \mathbf{q}' and \mathbf{q}'' (that is, by the product of the corresponding distribution functions).

Owing to its bosonic character, the creation of a phonon \mathbf{q} does not require that the state should be empty – moreover, the creation probability is even increased by the presence of existing phonons because of stimulated emission, yielding a factor $1 + g_\lambda(\mathbf{q})$. By taking into account the contributions of the other processes in Fig. 24.1,

$$\begin{aligned} \left(\frac{\partial g_\lambda}{\partial t} \right)_{\text{coll}} = \sum_{\lambda' \lambda''} \int \frac{d\mathbf{q}'}{(2\pi)^3} \{ & \frac{1}{2} W_{\mathbf{q}\mathbf{q}'} [g_{\lambda'}(\mathbf{q}') g_{\lambda''}(\mathbf{q} - \mathbf{q}') (1 + g_\lambda(\mathbf{q})) \\ & - g_\lambda(\mathbf{q}) (1 + g_{\lambda'}(\mathbf{q}')) (1 + g_{\lambda''}(\mathbf{q} - \mathbf{q}'))] \\ & + W_{\mathbf{q}'\mathbf{q}} [g_{\lambda'}(\mathbf{q}') (1 + g_\lambda(\mathbf{q})) (1 + g_{\lambda''}(\mathbf{q}' - \mathbf{q})) \\ & - g_\lambda(\mathbf{q}) g_{\lambda''}(\mathbf{q}' - \mathbf{q}) (1 + g_{\lambda'}(\mathbf{q}'))] \}. \end{aligned} \quad (24.2.29)$$

The factor $\frac{1}{2}$ in the first term is due to the indistinguishability of phonons: since the processes related by $\mathbf{q}' \leftrightarrow \mathbf{q} - \mathbf{q}'$ are identical, a twofold overcounting occurs in the \mathbf{q}' integral.

24.2.5 Coupled Electron–Phonon Systems

Because of the interaction between electrons and phonons, the two distribution functions are coupled. The collision term in the Boltzmann equation for the electron distribution function $f(\mathbf{r}, \mathbf{k}, t)$ contains the contributions of four kinds of process. The number of electrons with wave vector \mathbf{k} increases when an electron of wave vector $\mathbf{k}' = \mathbf{k} + \mathbf{q}$ emits a phonon of wave vector \mathbf{q} or absorbs one of wave vector $-\mathbf{q}$, and is thus scattered into the state of quantum number \mathbf{k} . On the other hand, the number of such electrons is reduced by the processes in which an electron of wave vector \mathbf{k} absorbs or emits a phonon. These possibilities are shown in Fig. 24.2.

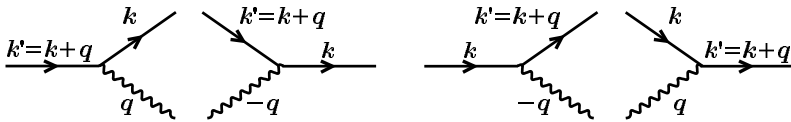


Fig. 24.2. Electron scattering processes with phonon emission and absorption that increase and decrease the number of electrons with wave vector \mathbf{k}

Consequently, the collision integral for electrons contains four terms. The collision term is proportional to the transition probabilities of the phonon-emission and -absorption processes. For the process in which an electron of wave vector \mathbf{k} absorbs one of the $n_\lambda(\mathbf{q})$ phonons of polarization λ and wave vector \mathbf{q} ,

$$W_{\mathbf{k}, \mathbf{q}, \lambda; \mathbf{k}'} = \frac{2\pi}{\hbar} \left| \langle \mathbf{k}', n_\lambda(\mathbf{q}) - 1 | \mathcal{H}_{\text{el-ph}} | \mathbf{k}, n_\lambda(\mathbf{q}) \rangle \right|^2 \delta(\varepsilon_{\mathbf{k}} + \hbar\omega_\lambda(\mathbf{q}) - \varepsilon_{\mathbf{k}'}) \delta_{\mathbf{k}+\mathbf{q}, \mathbf{k}'} . \quad (24.2.30)$$

The transition probabilities of other processes are similar in form. As the matrix element of the electron–phonon interaction is the same whether the electron emits or absorbs the phonon, after the separation of the factors granting energy and momentum conservation each process is proportional to

$$\begin{aligned} I_{\mathbf{k}, \mathbf{q}, \lambda} &= \frac{2\pi}{\hbar} \left| \langle \mathbf{k}' = \mathbf{k} + \mathbf{q}, n_\lambda(\mathbf{q}) - 1 | \mathcal{H}_{\text{el-ph}} | \mathbf{k}, n_\lambda(\mathbf{q}) \rangle \right|^2 \\ &= \frac{2\pi}{\hbar} \left| \langle \mathbf{k}' = \mathbf{k} - \mathbf{q}, n_\lambda(\mathbf{q}) + 1 | \mathcal{H}_{\text{el-ph}} | \mathbf{k}, n_\lambda(\mathbf{q}) \rangle \right|^2 . \end{aligned} \quad (24.2.31)$$

Of course, in phonon absorption and emission alike, the initial electron state must be occupied, while the final state that becomes occupied in the scattering must be initially empty according to the Pauli exclusion principle.

Similarly, the initial phonon state must be occupied in phonon-absorption processes, while in phonon-emission processes a factor $1 + g$ appears because of stimulated emission. Adding the scattering processes in their order in Fig. 24.2,

$$\begin{aligned} \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = \frac{1}{V} \sum_{\mathbf{k}' \mathbf{q} \lambda} \Big\{ & W_{\mathbf{k}'; \mathbf{k}, \mathbf{q}, \lambda} f(\mathbf{k}') [1 - f(\mathbf{k})] [1 + g_\lambda(\mathbf{q})] \\ & + W_{\mathbf{k}', -\mathbf{q}, \lambda; \mathbf{k}} f(\mathbf{k}') g_\lambda(-\mathbf{q}) [1 - f(\mathbf{k})] \\ & - W_{\mathbf{k}; \mathbf{k}', -\mathbf{q}, \lambda} f(\mathbf{k}) [1 - f(\mathbf{k}')] [1 + g_\lambda(-\mathbf{q})] \\ & - W_{\mathbf{k}, \mathbf{q}, \lambda; \mathbf{k}'} f(\mathbf{k}) g_\lambda(\mathbf{q}) [1 - f(\mathbf{k}')] \Big\}. \end{aligned} \quad (24.2.32)$$

The same scattering processes also contribute to the collision integral in the Boltzmann equation for phonons, since the phonon number is changed by phonon emission and absorption:

$$\begin{aligned} \left(\frac{\partial g_\lambda}{\partial t} \right)_{\text{coll}} = \frac{1}{V} \sum_{\mathbf{k} \mathbf{k}'} \Big\{ & W_{\mathbf{k}'; \mathbf{k}, \mathbf{q}, \lambda} f(\mathbf{k}') [1 - f(\mathbf{k})] [1 + g_\lambda(\mathbf{q})] \\ & - W_{\mathbf{k}, \mathbf{q}, \lambda; \mathbf{k}'} f(\mathbf{k}) g_\lambda(\mathbf{q}) [1 - f(\mathbf{k}')] \Big\}. \end{aligned} \quad (24.2.33)$$

To quantify the role of electron-phonon scattering, the coupled system of equations for the electron and phonon distribution functions needs to be solved. In thermal equilibrium the contributions of inscattering and outscattering processes cancel out, because when energy conservation is taken into account, $\varepsilon_{\mathbf{k}+\mathbf{q}} = \varepsilon_{\mathbf{k}} + \hbar\omega_\lambda(\mathbf{q})$ implies

$$f_0(\varepsilon_{\mathbf{k}+\mathbf{q}}) [1 - f_0(\varepsilon_{\mathbf{k}})] [1 + g_0(\omega_\lambda(\mathbf{q}))] = f_0(\varepsilon_{\mathbf{k}}) g_0(\omega_\lambda(\mathbf{q})) [1 - f_0(\varepsilon_{\mathbf{k}+\mathbf{q}})], \quad (24.2.34)$$

and similarly, $\varepsilon_{\mathbf{k}+\mathbf{q}} + \hbar\omega_\lambda(-\mathbf{q}) = \varepsilon_{\mathbf{k}}$ implies

$$f_0(\varepsilon_{\mathbf{k}+\mathbf{q}}) g_0(\omega_\lambda(-\mathbf{q})) [1 - f_0(\varepsilon_{\mathbf{k}})] = f_0(\varepsilon_{\mathbf{k}}) [1 - f_0(\varepsilon_{\mathbf{k}+\mathbf{q}})] [1 + g_0(\omega_\lambda(-\mathbf{q}))]. \quad (24.2.35)$$

This is the *principle of detailed balance* for individual processes. The collision integral vanishes unless an external perturbation drives the system out of thermal equilibrium. If the departure from equilibrium is small, and the occupation of electron states is expected to change only around the Fermi energy, the nonequilibrium distribution functions can be written as

$$\begin{aligned} f(\mathbf{k}) &= f_0(\mathbf{k}) - k_{\text{B}} T \frac{\partial f_0(\mathbf{k})}{\partial \varepsilon_{\mathbf{k}}} \chi(\mathbf{k}), \\ g_\lambda(\mathbf{q}) &= g_\lambda^0(\mathbf{q}) - \frac{k_{\text{B}} T}{\hbar} \frac{\partial g_0(\mathbf{q})}{\partial \omega_\lambda(\mathbf{q})} \phi_\lambda(\mathbf{q}). \end{aligned} \quad (24.2.36)$$

Writing out explicitly the derivative of the equilibrium distribution function,

$$\begin{aligned} f(\mathbf{k}) &= f_0(\mathbf{k}) + f_0(\mathbf{k}) (1 - f_0(\mathbf{k})) \chi(\mathbf{k}), \\ g_\lambda(\mathbf{q}) &= g_\lambda^0(\mathbf{q}) + g_\lambda^0(\mathbf{q}) [1 + g_\lambda^0(\mathbf{q})] \phi_\lambda(\mathbf{q}). \end{aligned} \quad (24.2.37)$$

By linearizing the collision integral in the small dimensionless quantities χ and ϕ , and making use of the property that the equilibrium phonon distribution function is even in \mathbf{q} , we find

$$\begin{aligned} \left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = & - \sum_{\mathbf{q}\lambda} I_{\mathbf{k},\mathbf{q},\lambda} f_0(\mathbf{k}) [1 - f_0(\mathbf{k} + \mathbf{q})] g_\lambda^0(\mathbf{q}) \\ & \times \{ \chi(\mathbf{k}) - \chi(\mathbf{k} + \mathbf{q}) + \phi_\lambda(\mathbf{q}) \} \delta(\varepsilon_{\mathbf{k}} + \hbar\omega_\lambda(\mathbf{q}) - \varepsilon_{\mathbf{k}+\mathbf{q}}) \\ & - \sum_{\mathbf{q}\lambda} I_{\mathbf{k},\mathbf{q},\lambda} f_0(\mathbf{k}) [1 - f_0(\mathbf{k} + \mathbf{q})] [1 + g_\lambda^0(\mathbf{q})] \\ & \times \{ \chi(\mathbf{k}) - \chi(\mathbf{k} + \mathbf{q}) - \phi_\lambda(-\mathbf{q}) \} \delta(\varepsilon_{\mathbf{k}} - \hbar\omega_\lambda(\mathbf{q}) - \varepsilon_{\mathbf{k}+\mathbf{q}}), \end{aligned} \quad (24.2.38)$$

and

$$\begin{aligned} \left(\frac{\partial g_\lambda}{\partial t}\right)_{\text{coll}} = & - \sum_{\mathbf{q}\lambda} I_{\mathbf{k},\mathbf{q},\lambda} f_0(\mathbf{k}) [1 - f_0(\mathbf{k} + \mathbf{q})] g_\lambda^0(\mathbf{q}) \\ & \times \{ \chi(\mathbf{k}) - \chi(\mathbf{k} + \mathbf{q}) + \phi_\lambda(\mathbf{q}) \} \delta(\varepsilon_{\mathbf{k}} + \hbar\omega_\lambda(\mathbf{q}) - \varepsilon_{\mathbf{k}+\mathbf{q}}). \end{aligned} \quad (24.2.39)$$

The system of equations is quite complicated even after this linearization. Instead of solving it, we usually study either the electron or phonon distribution function, and assume that the other subsystem is in thermal equilibrium.

24.3 Relaxation-Time Approximation

In the previous section we saw that the difficulty in solving the Boltzmann equation is rooted in the fact that the distribution function to be determined appears in the integrand of the collision term as well. Before turning to the general treatment of transport phenomena based on the Boltzmann equation, we shall first examine under what conditions the collision term can be interpreted in terms of a relaxation time, and where this treatment leads to. We shall then compare the results with those derived in the Drude and Sommerfeld models, where the finite relaxation time was assumed to be the same for each electron.

24.3.1 Relaxation Time

To introduce the relaxation time, we shall start with the impurity scattering formula (24.2.24). The collision term vanishes in thermal equilibrium, since the inscattering and outscattering processes compensate each other, that is,

$$W_{\mathbf{k}\mathbf{k}'} f_0(\mathbf{k}) [1 - f_0(\mathbf{k}')] = W_{\mathbf{k}'\mathbf{k}} f_0(\mathbf{k}') [1 - f_0(\mathbf{k})]. \quad (24.3.1)$$

This requirement, which formulates the condition of detailed balance for these processes, is customarily written as

$$W_{\mathbf{k}\mathbf{k}'} \exp[-\varepsilon_{\mathbf{k}}/k_{\text{B}}T] = W_{\mathbf{k}'\mathbf{k}} \exp[-\varepsilon_{\mathbf{k}'}/k_{\text{B}}T], \quad (24.3.2)$$

too. Naturally, $W_{\mathbf{k}\mathbf{k}'} = W_{\mathbf{k}'\mathbf{k}}$ for elastic scattering. Then

$$\begin{aligned} \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} &= \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}\mathbf{k}'} f_0(\mathbf{k}) [1 - f_0(\mathbf{k}')] \\ &\times \left[\frac{f(\mathbf{k}') [1 - f(\mathbf{k})]}{f_0(\mathbf{k}') [1 - f_0(\mathbf{k})]} - \frac{f(\mathbf{k}) [1 - f(\mathbf{k}')] }{f_0(\mathbf{k}) [1 - f_0(\mathbf{k}')] } \right]. \end{aligned} \quad (24.3.3)$$

Assuming that the departure $f_1 \equiv f - f_0$ from equilibrium is small,

$$\begin{aligned} \frac{f(\mathbf{k}') [1 - f(\mathbf{k})]}{f_0(\mathbf{k}') [1 - f_0(\mathbf{k})]} - \frac{f(\mathbf{k}) [1 - f(\mathbf{k}')] }{f_0(\mathbf{k}) [1 - f_0(\mathbf{k}')] } \\ = \frac{f_1(\mathbf{k}')}{f_0(\mathbf{k}') [1 - f_0(\mathbf{k}')] } - \frac{f_1(\mathbf{k})}{f_0(\mathbf{k}) [1 - f_0(\mathbf{k})] }. \end{aligned} \quad (24.3.4)$$

Making use of the formula

$$f_0(\mathbf{k}) [1 - f_0(\mathbf{k})] = -k_{\text{B}}T \frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \quad (24.3.5)$$

for the Fermi function, and rewriting f_1 in the previously used form

$$f_1(\mathbf{k}) = -k_{\text{B}}T \frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \chi(\mathbf{k}), \quad (24.3.6)$$

we have

$$\left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}\mathbf{k}'} f_0(\mathbf{k}) [1 - f_0(\mathbf{k}')] [\chi(\mathbf{k}') - \chi(\mathbf{k})]. \quad (24.3.7)$$

For elastic scattering, where $\varepsilon_{\mathbf{k}} = \varepsilon_{\mathbf{k}'}$,

$$\begin{aligned} \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} &= -k_{\text{B}}T \frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}\mathbf{k}'} [\chi(\mathbf{k}') - \chi(\mathbf{k})] \\ &= k_{\text{B}}T \frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \chi(\mathbf{k}) \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}\mathbf{k}'} \left[1 - \frac{\chi(\mathbf{k}')}{\chi(\mathbf{k})} \right] \\ &= -(f(\mathbf{k}) - f_0(\mathbf{k})) \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}\mathbf{k}'} \left[1 - \frac{\chi(\mathbf{k}')}{\chi(\mathbf{k})} \right]. \end{aligned} \quad (24.3.8)$$

The distribution function in a selected point \mathbf{r}, \mathbf{k} of the phase space usually depends on its value in other points; it is precisely for this reason that the collision term contains the integral of the distribution function. For elastic scattering, the collision integral could be cast in a simple form in which the departure from the equilibrium distribution is multiplied by a \mathbf{k} -dependent factor. To understand the physical meaning of the proportionality factor we

shall determine the variation of the number of particles due to collisions by another method.

Let $\tau(\mathbf{r}, \mathbf{k})$ be the mean time between collisions for a particle in the vicinity of point \mathbf{r}, \mathbf{k} of the phase space; in other words, let $1/\tau(\mathbf{r}, \mathbf{k})$ be the probability for the same particle to be scattered in unit time. Out of the dN_e particles in volume $d\mathbf{r} d\mathbf{k}/4\pi^3$ of the phase space

$$\frac{dt}{\tau(\mathbf{r}, \mathbf{k})} dN_e = \frac{dt}{\tau(\mathbf{r}, \mathbf{k})} f(\mathbf{r}, \mathbf{k}, t) \frac{d\mathbf{r} d\mathbf{k}}{4\pi^3} \quad (24.3.9)$$

are then scattered in time dt . These outscattering processes modify the distribution function by

$$df(\mathbf{r}, \mathbf{k}, t)_{\text{out}} = -\frac{dt}{\tau(\mathbf{r}, \mathbf{k})} f(\mathbf{r}, \mathbf{k}, t). \quad (24.3.10)$$

The analogous results for inscattering are just as straightforward to derive, only the two previously discussed fundamental conditions are required. The first condition is very natural: the collisions should not modify the distribution function in thermal equilibrium. The second is much less intuitive. It requires that the distribution after collisions should be independent of the state before the collisions – in other words, the collisions should erase the memory of the system. This implies that the strength of inscattering is independent of the instantaneous state of the local environment in phase space – that is, its departure from equilibrium is immaterial. Since inscattering and outscattering compensate each other in thermal equilibrium, we shall assume that the distribution function changes by

$$df(\mathbf{r}, \mathbf{k}, t)_{\text{in}} = \frac{dt}{\tau(\mathbf{r}, \mathbf{k})} f_0(\mathbf{r}, \mathbf{k}). \quad (24.3.11)$$

The total change due to collisions is then

$$\left(\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t} \right)_{\text{coll}} = -\frac{1}{\tau(\mathbf{r}, \mathbf{k})} [f(\mathbf{r}, \mathbf{k}, t) - f_0(\mathbf{r}, \mathbf{k})]. \quad (24.3.12)$$

If collisions were the only processes, the system would relax toward equilibrium with a characteristic time $\tau(\mathbf{r}, \mathbf{k})$ called the *relaxation time*.

Comparing this general expression with (24.3.8) leads to the following formula for the reciprocal of the relaxation time:

$$\frac{1}{\tau(\mathbf{k})} = \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}\mathbf{k}'} \left[1 - \frac{\chi(\mathbf{k}')}{\chi(\mathbf{k})} \right]. \quad (24.3.13)$$

Attention should be paid to a subtlety that turns out to be crucial in our later considerations: in the relaxation time (24.3.13), the transition probability $W_{\mathbf{k}\mathbf{k}'}$ is not simply integrated over each process (as would be if the inverse lifetime of a particle were to be calculated), but scattering processes are taken

into account by a weight factor that depends on the wave vectors \mathbf{k} and \mathbf{k}' . Therefore, the relaxation time τ is often called transport lifetime and sometimes denoted by τ_{tr} in order to distinguish it from the ordinary lifetime obtained from

$$\frac{1}{\tau(\mathbf{k})} = \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}\mathbf{k}'} . \quad (24.3.14)$$

Following the same steps, the collision term for phonons is often well approximated by expressing it in terms of the phonon relaxation time τ_{ph} as

$$\left(\frac{\partial g_{\lambda}(\mathbf{q})}{\partial t} \right)_{\text{coll}} = - \frac{g_{\lambda}(\mathbf{q}) - g_{\lambda}^0(\mathbf{q})}{\tau_{\text{ph}}(\mathbf{q})} . \quad (24.3.15)$$

The introduction of the relaxation time was based on the assumption of elastic scattering. It can be demonstrated that the relaxation-time approximation can also be used for quasielastic scattering, where the energy transfer is smaller than the thermal energy $k_{\text{B}}T$; otherwise the whole integral has to be considered. Looking back at (24.3.13), it should be noted that, through χ , the relaxation time also depends on the nonequilibrium distribution, and so it is not just a characteristic parameter of scattering. This observation also indicates the limitations of the relaxation-time approximation, even for elastic scattering.

24.3.2 Distribution Function in the Relaxation-Time Approximation

The most straightforward method to determine the distribution function is the direct integration of the Boltzmann equation. If no magnetic field is present and the driving forces are uniform – i.e., T is not constant in space but ∇T is –, this can be carried out without difficulty. When the collision term is written in the relaxation-time approximation, and the other terms on the right-hand side of the Boltzmann equation (24.2.21) are neglected – since, according to our assumptions, $\mathbf{B} = 0$, and the distribution function is spatially uniform –, the solution of the equation

$$- \left(- \frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \mathbf{v}_{\mathbf{k}} \cdot \left[-e \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) - \frac{\varepsilon_{\mathbf{k}} - \mu}{T} \nabla T \right] = - \frac{f(\mathbf{k}) - f_0(\mathbf{k})}{\tau(\varepsilon_{\mathbf{k}})} \quad (24.3.16)$$

is

$$f(\mathbf{k}) = f_0(\mathbf{k}) + \left(- \frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \tau(\varepsilon_{\mathbf{k}}) \mathbf{v}_{\mathbf{k}} \cdot \left[-e \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) - \frac{\varepsilon_{\mathbf{k}} - \mu}{T} \nabla T \right] . \quad (24.3.17)$$

Thus (16.3.27), which was derived using much simpler considerations, is recovered. This straightforward approach can no longer be used in the presence of a magnetic field. By applying CHAMBERS' method,² intuitive formulas are obtained that can be used in a wide range of applications.

² R. G. CHAMBERS, 1963.

Consider the phase-space volume element $d\mathbf{r} d\mathbf{k}$ around a point \mathbf{r}, \mathbf{k} at time t , and determine the electron trajectories $\mathbf{r}(t'), \mathbf{k}(t')$ for anterior times $t' < t$ by integrating the equation of motion backward in time from $\mathbf{r}(t), \mathbf{k}(t)$. These trajectories are shown in Fig. 24.3.

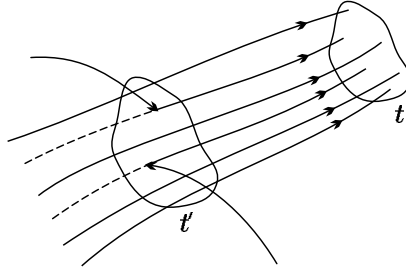


Fig. 24.3. Semiclassical trajectories of electrons running into a small neighborhood of a selected point of the phase space at time t

If there were no collisions, each electron that traverses one of these semiclassical trajectories would be in the selected region at time t . However, electrons trace out these trajectories only in the intervals between collisions. Some of the electrons are kicked off from them upon scattering, while others emerge on them after a collision. Eventually, those electrons reach the neighborhood of point \mathbf{r}, \mathbf{k} at time t that were scattered onto one of the trajectories at time $t' < t$ and did not undergo subsequent scattering before t .

The number of electrons that emerge on these trajectories after a collision during the time interval dt' around t' is given by

$$\frac{dt'}{\tau(\mathbf{r}(t'), \mathbf{k}(t'))} f_0(\mathbf{r}(t'), \mathbf{k}(t')) \frac{d\mathbf{r}' d\mathbf{k}'}{4\pi^3} \quad (24.3.18)$$

in the relaxation-time approximation. According to Liouville's theorem, $d\mathbf{r}' d\mathbf{k}' = d\mathbf{r} d\mathbf{k}$, thus the number of inscattered electrons is

$$\frac{dt'}{\tau(\mathbf{r}(t'), \mathbf{k}(t'))} f_0(\mathbf{r}(t'), \mathbf{k}(t')) \frac{d\mathbf{r} d\mathbf{k}}{4\pi^3}. \quad (24.3.19)$$

Denoting the probability that the particle does not undergo any further scattering by $P(\mathbf{r}, \mathbf{k}, t, t')$, the total number of electrons that arrive in the selected phase-space volume element at time t is given by the integral

$$dN = \int_{-\infty}^t \frac{dt'}{\tau(\mathbf{r}(t'), \mathbf{k}(t'))} f_0(\mathbf{r}(t'), \mathbf{k}(t')) P(\mathbf{r}, \mathbf{k}, t, t') \frac{d\mathbf{r} d\mathbf{k}}{4\pi^3}. \quad (24.3.20)$$

Comparison with (24.2.1), the defining equation of the distribution function, gives

$$f(\mathbf{r}, \mathbf{k}, t) = \int_{-\infty}^t dt' \frac{1}{\tau(\mathbf{r}(t'), \mathbf{k}(t'))} f_0(\mathbf{r}(t'), \mathbf{k}(t')) P(\mathbf{r}, \mathbf{k}, t, t'). \quad (24.3.21)$$

For simplicity, we keep only the time arguments:

$$f(t) = \int_{-\infty}^t dt' \frac{1}{\tau(t')} f_0(t') P(t, t'). \quad (24.3.22)$$

Since the collision probability in time dt' is dt'/τ , and that of collisionless propagation is $1 - dt'/\tau$, the probability $P(t, t')$ that no collision occurs from t' to t is

$$P(t, t') = P(t, t' + dt') \left[1 - \frac{dt'}{\tau(t')} \right], \quad (24.3.23)$$

and hence

$$\frac{\partial}{\partial t'} P(t, t') = \frac{P(t, t')}{\tau(t')}. \quad (24.3.24)$$

The solution that satisfies the initial condition $P(t, t) = 1$ is

$$P(t, t') = \exp \left(- \int_{t'}^t \frac{dt''}{\tau(t'')} \right). \quad (24.3.25)$$

Instead of using the explicit form of $P(t, t')$ in (24.3.22), it is more convenient to substitute (24.3.24) and perform an integration by parts. Since the probability that a particle never underwent collisions is zero [$P(t, -\infty) = 0$], we have

$$f(t) = \int_{-\infty}^t dt' f_0(t') \frac{\partial}{\partial t'} P(t, t') = f_0(t) - \int_{-\infty}^t dt' P(t, t') \frac{d}{dt'} f_0(t'). \quad (24.3.26)$$

As the t' -dependence appears through the arguments $\mathbf{r}(t')$ and $\mathbf{k}(t')$, the rules of implicit differentiation give

$$\frac{df_0(t')}{dt'} = \frac{\partial f_0(t')}{\partial \varepsilon_{\mathbf{k}}} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} \cdot \frac{d\mathbf{k}}{dt'} + \frac{\partial f_0(t')}{\partial T} \frac{\partial T}{\partial \mathbf{r}} \cdot \frac{d\mathbf{r}}{dt'} + \frac{\partial f_0(t')}{\partial \mu} \frac{\partial \mu}{\partial \mathbf{r}} \cdot \frac{d\mathbf{r}}{dt'}. \quad (24.3.27)$$

Since f_0 depends on the combination $[\varepsilon_{\mathbf{k}} - \mu(\mathbf{r})]/T(\mathbf{r})$, its derivatives can be expressed in terms of the derivatives with respect to the energy. Making use of the semiclassical equation of motion, we find

$$\begin{aligned} f(t) = f_0(t) + \int_{-\infty}^t dt' P(t, t') & \left(- \frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \\ & \times \mathbf{v}_{\mathbf{k}}(t') \cdot \left[-e\mathbf{E}(\mathbf{r}(t')) - \nabla \mu(\mathbf{r}(t')) - \frac{\varepsilon_{\mathbf{k}} - \mu}{T} \nabla T(\mathbf{r}(t')) \right]. \end{aligned} \quad (24.3.28)$$

This is the general form of the distribution function in the relaxation-time approximation. The magnetic field does not appear explicitly, but it does implicitly, since it has strong influence on the semiclassical electron trajectories.

If the electric field and the temperature gradient are weak, and linear effects are considered, $P(t, t')$, which depends on the collisions, can often be approximated by the formulas obtained for $\mathbf{E} = 0$ and $\nabla T = 0$. In a uniform field nothing depends explicitly on $\mathbf{r}(t')$, only implicitly, through $\mathbf{k}(t')$. It is customary to assume that the relaxation time depends on \mathbf{k} only through $\varepsilon_{\mathbf{k}}$. Since $\varepsilon_{\mathbf{k}}$ is constant in a uniform magnetic field, the integral in $P(t, t')$ can be evaluated:

$$P(t, t') = e^{-(t-t')/\tau(\varepsilon_{\mathbf{k}})}, \quad (24.3.29)$$

and

$$\begin{aligned} f(t) = f_0(t) + \int_{-\infty}^t dt' e^{-(t-t')/\tau(\varepsilon_{\mathbf{k}})} & \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \\ & \times \mathbf{v}_{\mathbf{k}}(t') \cdot \left[-e \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) - \frac{\varepsilon_{\mathbf{k}} - \mu}{T} \nabla T \right]. \end{aligned} \quad (24.3.30)$$

In terms of the quantity

$$\mathbf{w}_{\mathbf{k}}(t) = \frac{1}{\tau(\varepsilon_{\mathbf{k}})} \int_{-\infty}^t dt' e^{-(t-t')/\tau(\varepsilon_{\mathbf{k}})} \mathbf{v}_{\mathbf{k}}(t'), \quad (24.3.31)$$

the distribution function can be written as

$$f(t) = f_0(t) + \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \tau(\varepsilon_{\mathbf{k}}) \mathbf{w}_{\mathbf{k}}(t) \cdot \left[-e \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) - \frac{\varepsilon_{\mathbf{k}} - \mu}{T} \nabla T \right]. \quad (24.3.32)$$

When no external magnetic field is present, and the driving forces are uniform, the drift velocity is constant in time and, according to (24.3.31), $\mathbf{w}_{\mathbf{k}} = \mathbf{v}_{\mathbf{k}}$. The stationary distribution function is therefore

$$f(\mathbf{k}) = f_0(\mathbf{k}) + \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \tau(\varepsilon_{\mathbf{k}}) \mathbf{v}_{\mathbf{k}} \cdot \left[-e \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) - \frac{\varepsilon_{\mathbf{k}} - \mu}{T} \nabla T \right]. \quad (24.3.33)$$

Note that this is the same as (24.3.17), which was obtained for the same situation. In the presence of a magnetic field, where the velocity changes on account of moving in a circular orbit, the relationship between the results of the two approaches is less conspicuous. Depending on the character of the particular situation, we shall use either form below.

24.3.3 DC Conductivity

According to the foregoing, in the absence of a magnetic field and a temperature gradient, when \mathbf{E} is constant, the distribution function is given by

$$f(\mathbf{k}) = f_0(\mathbf{k}) - e(\mathbf{E} \cdot \mathbf{v}_{\mathbf{k}}) \tau(\varepsilon_{\mathbf{k}}) \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right). \quad (24.3.34)$$

This is the same as our previous result (16.3.17) obtained by assuming that the stationary distribution function can be derived from the Fermi function by shifting the energy in its argument by $e\tau\mathbf{E}/\hbar$, the energy gained from the electric field. As (24.3.34) shows, the approach based on the Boltzmann equation asserts that the same formula is applicable to Bloch electrons, too.

Writing the current density carried by electrons in its customary form, and noting that the current vanishes in thermal equilibrium,

$$\mathbf{j} = -e \frac{1}{V} \sum_{\mathbf{k}, \sigma} \mathbf{v}_{\mathbf{k}} [f(\mathbf{k}) - f_0(\mathbf{k})] = -e \int \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}_{\mathbf{k}} [f(\mathbf{k}) - f_0(\mathbf{k})]. \quad (24.3.35)$$

By separating the part of the distribution function that is proportional to the electric field, the conductivity tensor is found to be

$$\boldsymbol{\sigma} = e^2 \int \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}_{\mathbf{k}} \circ \mathbf{v}_{\mathbf{k}} \tau(\varepsilon_{\mathbf{k}}) \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right), \quad (24.3.36)$$

where $\mathbf{v}_{\mathbf{k}} \circ \mathbf{v}_{\mathbf{k}}$ denotes the diadic product of the two vectors. This tensor exhibits the symmetries of the crystal lattice. In cubic crystals $\sigma_{\alpha\beta} = \delta_{\alpha\beta} \sigma$, and thus the conductivity can be specified by a scalar. For lower symmetries, \mathbf{j} and \mathbf{E} are not necessarily parallel, and, depending on the symmetry, off-diagonal tensor elements may also appear.

Because of the derivative of the Fermi function only those electrons contribute that are close to ε_F , within a region of width $k_B T$. When the conductivity at $T = 0$ is considered, the factor $\tau(\varepsilon_F)$ can be taken outside the integral. Making use of

$$\mathbf{v}_{\mathbf{k}} \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) = -\frac{1}{\hbar} \frac{\partial f_0(\varepsilon_{\mathbf{k}})}{\partial \mathbf{k}}, \quad (24.3.37)$$

the formula for the conductivity is

$$\boldsymbol{\sigma} = -\frac{1}{\hbar} e^2 \tau(\varepsilon_F) \int \frac{d\mathbf{k}}{4\pi^3} \mathbf{v}_{\mathbf{k}} \circ \frac{\partial f_0(\varepsilon_{\mathbf{k}})}{\partial \mathbf{k}}. \quad (24.3.38)$$

Integrating by parts, and assuming that the dispersion relation can be specified in terms of a scalar effective mass, at zero temperature we have

$$\sigma_0 = e^2 \tau(\varepsilon_F) \int \frac{d\mathbf{k}}{4\pi^3} \frac{1}{\hbar} \frac{\partial \mathbf{v}_{\mathbf{k}}}{\partial \mathbf{k}} f_0(\varepsilon_{\mathbf{k}}) = e^2 \tau(\varepsilon_F) \int_{\text{occupied}} \frac{d\mathbf{k}}{4\pi^3} \frac{1}{m_{\mathbf{k}}^*}. \quad (24.3.39)$$

If the effective mass is independent of \mathbf{k} , the Drude formula

$$\sigma_0 = \frac{n_e e^2 \tau}{m^*} \quad (24.3.40)$$

is recovered, with the sole difference that the electron mass is replaced by the effective mass. A perfectly intuitive meaning can be given to n_e : it is the number (density) of electrons in the partially filled conduction band, while τ is the transport relaxation time of electrons on the Fermi surface.

If the integral in the conductivity is performed over the entire Brillouin zone rather than the occupied states, it vanishes, as completely filled bands do not contribute to the current. Therefore, a negative sign aside, the integration could be done over the empty states as well, leading to

$$\sigma_0 = e^2 \tau (\varepsilon_F) \int_{\text{empty}} \frac{d\mathbf{k}}{4\pi^3} \left(-\frac{1}{m_{\mathbf{k}}^*} \right). \quad (24.3.41)$$

Since the electron and hole masses are defined to be opposite in sign, the same form is obtained for the current and conductivity as above, provided the latter is expressed in terms of the effective hole mass m_h^* :

$$\sigma_0 = \frac{n_h e^2 \tau}{m_h^*}, \quad (24.3.42)$$

where n_h is the number of holes per unit volume.

24.3.4 AC and Optical Conductivity

To determine the AC conductivity, we start with the distribution function formula (24.3.30) obtained using Chambers' method. In an electric field $\mathbf{E}(t) = \mathbf{E}(\omega) e^{-i\omega t}$ of frequency ω , the integral over the semiclassical trajectory of electrons can be evaluated:

$$\begin{aligned} f(\mathbf{k}, t) &= f_0(\mathbf{k}) + \int_{-\infty}^t dt' e^{-(t-t')/\tau(\varepsilon_{\mathbf{k}})} \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) (-e) \mathbf{v}_{\mathbf{k}}(t') \cdot \mathbf{E}(\omega) e^{-i\omega t'} \\ &= f_0(\mathbf{k}) - e^{-i\omega t} \int_{-\infty}^t dt' e^{-(t-t')[1/\tau(\varepsilon_{\mathbf{k}}) - i\omega]} \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) e \mathbf{v}_{\mathbf{k}}(t') \cdot \mathbf{E}(\omega) \\ &= f_0(\mathbf{k}) - e^{-i\omega t} \frac{1}{1/\tau(\varepsilon_{\mathbf{k}}) - i\omega} \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) e \mathbf{v}_{\mathbf{k}} \cdot \mathbf{E}(\omega). \end{aligned} \quad (24.3.43)$$

Expressing the current density through this formula, the frequency-dependent (AC) conductivity is

$$\sigma_{\alpha\beta}(\omega) = e^2 \int \frac{d\mathbf{k}}{4\pi^3} v_{\mathbf{k}}^{\alpha} v_{\mathbf{k}}^{\beta} \frac{1}{1/\tau(\varepsilon_{\mathbf{k}}) - i\omega} \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right). \quad (24.3.44)$$

If the relaxation time is independent of the energy, and the system is isotropic or exhibits cubic symmetry, we have

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}, \quad (24.3.45)$$

just like in the Drude model, where

$$\sigma_0 = e^2 \int \frac{d\mathbf{k}}{4\pi^3} \frac{1}{2} v_{\mathbf{k}}^2 \tau \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right). \quad (24.3.46)$$

This means that when the periodic potential of the lattice is taken into account, then the same results are obtained for the optical properties of metals and the role of the plasma frequency in the relaxation-time approximation as in the classical model of free electrons.

When σ_0 is written in the Drude form, the mass that appears in the denominator is neither the electron mass nor the dynamical effective mass of Bloch electrons but a new parameter called the *optical mass*:

$$\sigma_0 = n_e e^2 \tau / m_{\text{opt}}, \quad (24.3.47)$$

where the inverse of the optical mass is given by

$$m_{\text{opt}}^{-1} = \frac{1}{3n_e} \int \frac{d\mathbf{k}}{4\pi^3} v_{\mathbf{k}}^2 \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right). \quad (24.3.48)$$

Following the same steps as for the density of states, we now decompose the \mathbf{k} -space integral into integrals over the constant-energy surfaces and the component of \mathbf{k} that is perpendicular to them,

$$\int d\mathbf{k} = \int d\varepsilon \int \frac{dS}{\hbar v_{\mathbf{k}}}, \quad (24.3.49)$$

which gives

$$m_{\text{opt}}^{-1} = \frac{1}{12\pi^3 \hbar n_e} \int_{S(\varepsilon_F)} v_{\mathbf{k}} dS, \quad (24.3.50)$$

where the integral is over the Fermi surface. For free electrons m_e is recovered, but in general m_{opt} is different from the dynamical effective mass.

24.3.5 General Form of Transport Coefficients

In the foregoing the distribution function was determined in two different ways for uniform driving forces and zero magnetic field. It was also mentioned that the results given in (24.3.17) and (24.3.33) are formally identical to the free-electron formula (16.3.27). The only differences are that $\varepsilon_{\mathbf{k}}$ is now taken from band-structure calculations (instead of the simple isotropic and quadratic dispersion relation for free electrons), and the electron velocity is the group velocity derived from the dispersion relation. Moreover, the relaxation time may depend on $\varepsilon_{\mathbf{k}}$.

Using this distribution function in the formulas for the electric and heat currents, the kinetic coefficients defined by the relations

$$\begin{aligned} \mathbf{j} &= L_{11} \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) + L_{12} \left(-\frac{\nabla T}{T} \right), \\ \mathbf{j}_Q &= L_{21} \left(\mathbf{E} + \frac{\nabla \mu}{e} \right) + L_{22} \left(-\frac{\nabla T}{T} \right) \end{aligned} \quad (24.3.51)$$

are tensor quantities that exhibit the symmetries of the crystal itself:

$$\begin{aligned} L_{11}^{\alpha\beta} &= e^2 \int \frac{d\mathbf{k}}{4\pi^3} \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \tau(\varepsilon_{\mathbf{k}}) v_{\alpha}(\mathbf{k}) v_{\beta}(\mathbf{k}), \\ L_{12}^{\alpha\beta} &= L_{21}^{\alpha\beta} = -e \int \frac{d\mathbf{k}}{4\pi^3} \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \tau(\varepsilon_{\mathbf{k}}) v_{\alpha}(\mathbf{k}) v_{\beta}(\mathbf{k}) (\varepsilon_{\mathbf{k}} - \mu), \\ L_{22}^{\alpha\beta} &= \int \frac{d\mathbf{k}}{4\pi^3} \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \tau(\varepsilon_{\mathbf{k}}) v_{\alpha}(\mathbf{k}) v_{\beta}(\mathbf{k}) (\varepsilon_{\mathbf{k}} - \mu)^2. \end{aligned} \quad (24.3.52)$$

The \mathbf{k} -space integral can be decomposed into an integral over the constant-energy surface and an energy integral. By introducing

$$\sigma_{\alpha\beta}(\varepsilon) = \frac{e^2 \tau(\varepsilon)}{4\pi^3} \int_{\varepsilon_{\mathbf{k}}=\varepsilon} \frac{dS}{|\nabla \varepsilon_{\mathbf{k}}|} v_{\alpha}(\mathbf{k}) v_{\beta}(\mathbf{k}), \quad (24.3.53)$$

the kinetic coefficients can be written as

$$\begin{aligned} L_{11}^{\alpha\beta} &= \int d\varepsilon \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \sigma_{\alpha\beta}(\varepsilon), \\ L_{12}^{\alpha\beta} &= L_{21}^{\alpha\beta} = -\frac{1}{e} \int d\varepsilon \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) (\varepsilon - \mu) \sigma_{\alpha\beta}(\varepsilon), \\ L_{22}^{\alpha\beta} &= \frac{1}{e^2} \int d\varepsilon \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) (\varepsilon - \mu)^2 \sigma_{\alpha\beta}(\varepsilon). \end{aligned} \quad (24.3.54)$$

Assuming that close to the Fermi surface $\sigma_{\alpha\beta}(\varepsilon)$ varies slowly, the Sommerfeld expansion can be applied. Keeping only the leading term, the value of $\sigma_{\alpha\beta}(\varepsilon)$ at the Fermi energy gives directly the conductivity tensor.

Applying the Sommerfeld expansion to L_{22} , too, we have

$$L_{22}^{\alpha\beta} = \frac{\pi^2}{3e^2} (k_B T)^2 \sigma_{\alpha\beta}(\varepsilon_F). \quad (24.3.55)$$

Since the leading term of the thermal conductivity is $\lambda = L_{22}/T$, the Wiedemann–Franz law, which was derived for free electrons in Section 16.1.3, applies also to Bloch electrons in the semiclassical approximation.

24.3.6 Hall Effect

If the effect of the magnetic field on electrons were taken into account in (24.3.34) by replacing \mathbf{E} by $\mathbf{E} + \mathbf{v}_\mathbf{k} \times \mathbf{B}$, as in the Lorentz force, nothing would change, since this combination is multiplied by $\mathbf{v}_\mathbf{k}$. However, it is well known from classical physics that crossed electric and magnetic fields give rise to the Hall effect. To derive it in our present framework, we must either solve the Boltzmann equation more accurately, or start with Chambers' formula of the distribution function, exploiting that electrons in a magnetic field move in cyclotron orbits semiclassically. We shall see both approaches below.

We start with the Boltzmann equation (24.2.21), and apply it to the case of crossed uniform electric and magnetic fields. If the collision term is treated in the relaxation-time approximation, we have

$$e\mathbf{E} \cdot \mathbf{v}_\mathbf{k} \left(-\frac{\partial f_0}{\partial \varepsilon_\mathbf{k}} \right) = -\frac{f_1}{\tau} + \frac{e}{\hbar} (\mathbf{v}_\mathbf{k} \times \mathbf{B}) \cdot \frac{\partial f_1}{\partial \mathbf{k}}. \quad (24.3.56)$$

The solution can be sought in the form

$$f_1 \equiv f - f_0 = -e \left(-\frac{\partial f_0}{\partial \varepsilon_\mathbf{k}} \right) \tau \mathbf{v}_\mathbf{k} \cdot \mathbf{A}, \quad (24.3.57)$$

where \mathbf{A} is yet to be determined. Then, following the steps of Section 24.3.3, the particularly simple relation

$$\mathbf{j} = \sigma_0 \mathbf{A} \quad (24.3.58)$$

is obtained in the isotropic case, where σ_0 is the usual Drude conductivity.

Substituting (24.3.57) into the right-hand side of (24.3.56), the derivative of f_1 with respect to \mathbf{k} can be calculated using the relation $\mathbf{v}_\mathbf{k} = \hbar \mathbf{k} / m^*$, which is valid in the effective-mass approximation. We then have

$$e\mathbf{E} \cdot \mathbf{v}_\mathbf{k} \left(-\frac{\partial f_0}{\partial \varepsilon_\mathbf{k}} \right) = e \left(-\frac{\partial f_0}{\partial \varepsilon_\mathbf{k}} \right) \mathbf{v}_\mathbf{k} \cdot \mathbf{A} - \frac{e^2 \tau}{m^*} \left(-\frac{\partial f_0}{\partial \varepsilon_\mathbf{k}} \right) (\mathbf{v}_\mathbf{k} \times \mathbf{B}) \cdot \mathbf{A}, \quad (24.3.59)$$

which implies

$$\mathbf{E} \cdot \mathbf{v}_\mathbf{k} = \mathbf{v}_\mathbf{k} \cdot \mathbf{A} - \frac{e\tau}{m^*} (\mathbf{v}_\mathbf{k} \times \mathbf{B}) \cdot \mathbf{A}. \quad (24.3.60)$$

By rearranging the scalar triple product in the second term of the right-hand side, it is readily seen that the equation can be satisfied for any $\mathbf{v}_\mathbf{k}$ only when

$$\mathbf{E} = \mathbf{A} - \frac{e\tau}{m^*} (\mathbf{B} \times \mathbf{A}). \quad (24.3.61)$$

Whatever the relative orientation of the electric and magnetic fields, this equation can be solved. The components of \mathbf{E} , \mathbf{A} , and \mathbf{j} that are parallel to the magnetic field satisfy

$$\mathbf{E}_\parallel = \mathbf{A}_\parallel, \quad (24.3.62)$$

and thus

$$\mathbf{j}_{\parallel} = \sigma_0 \mathbf{E}_{\parallel}. \quad (24.3.63)$$

The magnetic field does not affect the parallel component of the current. The resistivity is the same as in the absence of the magnetic field. There is no longitudinal magnetoresistance in isotropic metals with a spherical Fermi surface.

As for the components that are perpendicular to the magnetic field: according to (24.3.61), \mathbf{A}_{\perp} is also perpendicular to the magnetic field, and is thus in the plane spanned by the vectors \mathbf{E}_{\perp} and $\mathbf{B} \times \mathbf{E}_{\perp}$. By seeking it in the form $\mathbf{A}_{\perp} = a\mathbf{E}_{\perp} + b(\mathbf{B} \times \mathbf{E}_{\perp})$, and substituting that into (24.3.61), it follows immediately that

$$\mathbf{A}_{\perp} = \frac{\mathbf{E}_{\perp} + \frac{e\tau}{m^*} \mathbf{B} \times \mathbf{E}_{\perp}}{1 + \left(\frac{e\tau}{m^*}\right)^2 B^2}. \quad (24.3.64)$$

Substituting this into (24.3.58),

$$\mathbf{j}_{\perp} = \sigma_0 \frac{\mathbf{E}_{\perp} + \frac{e\tau}{m^*} \mathbf{B} \times \mathbf{E}_{\perp}}{1 + \left(\frac{e\tau}{m^*}\right)^2 B^2} \quad (24.3.65)$$

is obtained. Thus in crossed electric and magnetic fields the current flow is not parallel to the electric field: a component that is perpendicular to both the electric and magnetic fields is also present.

This can be cast in another form by eliminating \mathbf{A} from (24.3.61):

$$\mathbf{E} = \frac{1}{\sigma_0} \mathbf{j} - \frac{e\tau}{m^*} \mathbf{B} \times \frac{1}{\sigma_0} \mathbf{j} = \varrho_0 \mathbf{j} - \frac{e\tau}{m^*} \varrho_0 \mathbf{B} \times \mathbf{j}. \quad (24.3.66)$$

When the applied magnetic field is perpendicular to the current, the electric field acquires a new component that is perpendicular both to the current and the magnetic field:

$$E_H = -\frac{e\tau}{m^*} \varrho_0 B j. \quad (24.3.67)$$

Choosing the z -axis along the magnetic, and the y -axis along the electric field, the Hall coefficient is defined by

$$R_H = \frac{E_y}{j_x B} = \frac{\varrho_{yx}(B)}{B}. \quad (24.3.68)$$

Note that for nonspherical Fermi surfaces $\varrho_{yx}(B=0)$ can be finite. The proper definition of the Hall coefficient is then

$$R_H = \frac{1}{2B} [\varrho_{yx}(B) - \varrho_{yx}(-B)]. \quad (24.3.69)$$

In our case the Hall coefficient is

$$R_H = -\frac{e\tau}{m^*} \varrho_0 = -\frac{e\tau}{m^*} \frac{m^*}{n_e e^2 \tau} = -\frac{1}{n_e e}. \quad (24.3.70)$$

The calculation is similar for hole conduction. In line with our previous observation that holes behave as positively charged particles,

$$R_H = \frac{1}{n_h e} \quad (24.3.71)$$

is obtained for the Hall coefficient. This explains why the Hall coefficient measured in experiments is not always negative – even though the Sommerfeld model would imply that.

24.3.7 Alternative Treatment of Transport in Magnetic Fields

In the previous subsection we examined how an applied magnetic field affected transport properties for systems with a spherical Fermi surface. In the more general case the transport coefficients can be determined using Chambers' method. Before turning to this discussion, we shall demonstrate how the previously derived results can be recovered in Chambers' approach.

According to (24.3.32), when both electric and magnetic fields are present, and the temperature is uniform (thus $\nabla\mu = 0$), we have

$$f(t) = f_0(t) - e \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \tau(\varepsilon_{\mathbf{k}}) \mathbf{w}_{\mathbf{k}}(t) \cdot \mathbf{E}, \quad (24.3.72)$$

where $\mathbf{w}_{\mathbf{k}}(t)$ can be calculated from the velocity of electrons by integrating over the trajectory:

$$\mathbf{w}_{\mathbf{k}}(t) = \frac{1}{\tau(\varepsilon_{\mathbf{k}})} \int_{-\infty}^t dt' e^{-(t-t')/\tau(\varepsilon_{\mathbf{k}})} \mathbf{v}_{\mathbf{k}}(t'). \quad (24.3.73)$$

When the Fermi surface is spherical, and a z -directed magnetic field is applied, the electron moves in a helical path, and its projection on the xy -plane is a circular motion of angular frequency ω_c . If the velocity is given by $v_{\mathbf{k}}^x = v_{\mathbf{k}\perp} \cos \phi$, $v_{\mathbf{k}}^y = v_{\mathbf{k}\perp} \sin \phi$, $v_{\mathbf{k}}^z = v_{\mathbf{k}\parallel}$ at $t = 0$, then at an arbitrary time t it is

$$\begin{aligned} \mathbf{v}_{\mathbf{k}}(t) &= [v_{\mathbf{k}\perp} \cos(\omega_c t + \phi), v_{\mathbf{k}\perp} \sin(\omega_c t + \phi), v_{\mathbf{k}\parallel}] \\ &= [v_{\mathbf{k}}^x \cos \omega_c t - v_{\mathbf{k}}^y \sin \omega_c t, v_{\mathbf{k}}^x \sin \omega_c t + v_{\mathbf{k}}^y \cos \omega_c t, v_{\mathbf{k}\parallel}]. \end{aligned} \quad (24.3.74)$$

Substituting this back into the above formula for $\mathbf{w}_{\mathbf{k}}$, and making use of the relations

$$\frac{1}{\tau} \int_{-\infty}^0 dt' e^{t'/\tau} \begin{Bmatrix} \cos \omega_c t' \\ \sin \omega_c t' \end{Bmatrix} = \frac{1}{1 + (\omega_c \tau)^2} \begin{Bmatrix} 1 \\ -\omega_c \tau \end{Bmatrix}, \quad (24.3.75)$$

we have

$$\mathbf{w}_{\mathbf{k}} = \left\{ \frac{v_{\mathbf{k}}^x}{1 + (\omega_c \tau)^2} + \frac{v_{\mathbf{k}}^y \omega_c \tau}{1 + (\omega_c \tau)^2}, \frac{v_{\mathbf{k}}^y}{1 + (\omega_c \tau)^2} - \frac{v_{\mathbf{k}}^x \omega_c \tau}{1 + (\omega_c \tau)^2}, v_{\mathbf{k}\parallel}(\mathbf{k}) \right\}. \quad (24.3.76)$$

Using this formula in the distribution function to determine the current, the conductivity tensor is

$$\sigma_{\alpha\beta}(B) = \sigma_0 \begin{pmatrix} \frac{1}{1 + (\omega_c \tau)^2} & \frac{-\omega_c \tau}{1 + (\omega_c \tau)^2} & 0 \\ \frac{\omega_c \tau}{1 + (\omega_c \tau)^2} & \frac{1}{1 + (\omega_c \tau)^2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (24.3.77)$$

where $\sigma_0 = n_e e^2 \tau / m^*$. By inverting it,

$$\varrho_{\alpha\beta}(B) = \varrho_0 \begin{pmatrix} 1 & \omega_c \tau & 0 \\ -\omega_c \tau & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (24.3.78)$$

is obtained for the resistivity tensor. The off-diagonal elements give the Hall coefficient, and the previous result is duly recovered. The diagonal terms are, on the other hand, independent of the magnetic field. This means that the current along the electric field is the same whether or not a magnetic field is present.

24.3.8 Magnetoresistance

The previous results are valid only for spherical Fermi surfaces. For nonspherical Fermi surfaces the conductivity can substantially change on the application of a magnetic field, since electrons no longer traverse circular orbits in \mathbf{k} -space – and, consequently, in real space, either. In many cases their orbits are not even closed.

When the inverse of the conductivity tensor, the resistivity tensor

$$\varrho_{\alpha\beta}(\mathbf{B}) = [\sigma^{-1}(\mathbf{B})]_{\alpha\beta} \quad (24.3.79)$$

is examined in the presence of a z -directed magnetic field, $\varrho_{xx}(B)$ and $\varrho_{yy}(B)$ specify the transverse, and $\varrho_{zz}(B)$ the longitudinal magnetoresistance.

Suppose that electrons move in a closed orbit in a section of a nonspherical Fermi surface. To obtain generally valid results in strong fields, symmetry

considerations need to be applied. When the field is so strong that the period of the cyclotron orbit is much shorter than the mean time between collisions, the exponential factor in the integral for $\mathbf{w}_{\mathbf{k}}$ varies little over a period T_c , and so

$$\mathbf{w}_{\mathbf{k}} \propto \int_0^{T_c} dt \mathbf{v}_{\mathbf{k}}(t). \quad (24.3.80)$$

The integral over the closed orbit vanishes for the velocity components perpendicular to the magnetic field; only the integral of the field-directed z component survives. Thus in the $B \rightarrow \infty$ limit σ_{zz} is the single nonvanishing component of the conductivity tensor.

In large but finite magnetic fields the magnetic-field-dependent corrections can be expanded into a power series of $1/B$,

$$\sigma_{\alpha\beta}(B) = A_{\alpha\beta} + \frac{1}{B}B_{\alpha\beta} + \frac{1}{B^2}C_{\alpha\beta} + \dots \quad (24.3.81)$$

Because of the Onsager relation, the condition

$$\sigma_{\alpha\beta}(B) = \sigma_{\beta\alpha}(-B) \quad (24.3.82)$$

must be satisfied. Applying it to the series above, we have

$$A_{\alpha\beta} + \frac{1}{B}B_{\alpha\beta} + \frac{1}{B^2}C_{\alpha\beta} + \dots = A_{\beta\alpha} - \frac{1}{B}B_{\beta\alpha} + \frac{1}{B^2}C_{\beta\alpha} + \dots \quad (24.3.83)$$

Comparison of the terms of the same order shows that each diagonal element must be either a constant or proportional to $1/B^2$. If the Fermi surface is closed, then, according to our previous considerations, only the zz component can be a constant. On the other hand, the off-diagonal elements can be of order $1/B$ or smaller. Therefore,

$$\sigma_{\alpha\beta}(B) = \begin{pmatrix} \frac{C_{xx}}{B^2} & \frac{B_{xy}}{B} & \frac{B_{xz}}{B} \\ -\frac{B_{xy}}{B} & \frac{C_{yy}}{B^2} & \frac{B_{yz}}{B} \\ -\frac{B_{xz}}{B} & -\frac{B_{yz}}{B} & A_{zz} \end{pmatrix}. \quad (24.3.84)$$

By inverting this matrix,

$$\varrho_{xx} \sim \frac{C_{yy}A_{zz} + B_{yz}^2}{A_{zz}B_{xy}^2} \quad (24.3.85)$$

in leading order. A similar expression holds for ϱ_{yy} . They show that the transverse magnetoresistance tends to a finite value.

The situation is radically different when the electrons move in open trajectories. If the \mathbf{k} -space orbit does not close in the k_y -direction, then the x

component of the velocity does not average out to zero in the high-field limit, and only those components of $\sigma_{\alpha\beta}(B)$ vanish in this limit for which either α or β is equal to y . Thus we have

$$\sigma_{\alpha\beta}(B) = \begin{pmatrix} A_{xx} & \frac{B_{xy}}{B} & A_{xz} \\ -\frac{B_{xy}}{B} & \frac{C_{yy}}{B^2} & \frac{B_{yz}}{B} \\ -A_{xz} & -\frac{B_{yz}}{B} & A_{zz} \end{pmatrix}. \quad (24.3.86)$$

Once again, ρ_{xx} becomes saturated – but ρ_{yy} does not: $\rho_{yy} \sim B^2$.

By rotating the sample relative to the magnetic field direction, and measuring the variation of the resistivity, one can infer the directions along which the electron orbits are closed and open. This provides information about the topology of the cross sections of the Fermi surface. Figure 24.4(a) shows the angular dependence of the resistivity of β -(BEDT-TTF) $_2$ I $_3$ when the magnetic field direction is rotated in the plane perpendicular to a plane of high conductivity. Part (b) shows the calculated angular dependence of ρ_{zz} for the highly anisotropic Fermi surface illustrated in the top left part.

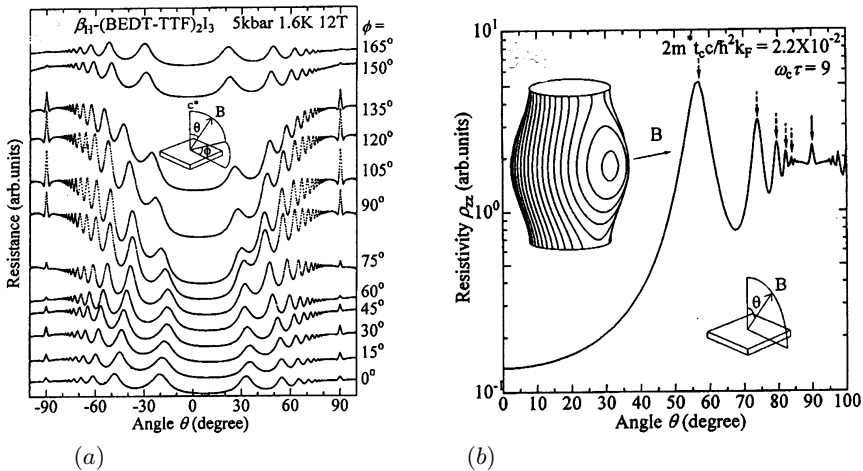


Fig. 24.4. (a) Variations of the magnetoresistance of the quasi-two-dimensional β -(BEDT-TTF) $_2$ I $_3$ as the magnetic field is rotated in a plane perpendicular to the conducting plane. (b) Electron orbits on the quasi-two-dimensional Fermi surface in a magnetic field and the calculated angular dependence of the resistance ρ_{zz} [Reprinted with permission from N. Hanasaki et al., *Phys. Rev. B* **57**, 1336 (1998). ©1998 by the American Physical Society]

24.4 Transport Coefficients in Metals and Semiconductors

In the previous sections we ignored the microscopic origin of scattering processes, and studied transport phenomena in the relaxation-time approximation. We shall now examine how individual scattering processes – such as scattering by impurities and crystal defects, interaction with lattice vibrations (phonons), and electron–electron interactions – modify the transport coefficients. We shall also discuss the applicability of the relaxation-time approximation.

Studying individual scattering processes separately is justified if they do not interfere. *Matthiessen's rule*³ is the formulation of the empirical observation that the resistivities due to different scattering processes – such as ϱ_{imp} , due to impurity scattering, and $\varrho_{\text{el-ph}}$, due to the electron–phonon interaction – add up:

$$\varrho = \varrho_{\text{imp}} + \varrho_{\text{el-ph}}. \quad (24.4.1)$$

For the relaxation times this implies reciprocal additivity:

$$\frac{1}{\tau} = \frac{1}{\tau_{\text{imp}}} + \frac{1}{\tau_{\text{el-ph}}}. \quad (24.4.2)$$

Even though deviations from Matthiessen's rule are not rare, assuming its validity allows us to separate experimental results into the contributions of individual scattering processes.

24.4.1 Scattering of Electrons by Impurities

Assuming that the sample contains a small number (n_i) of randomly distributed immobile impurities, the quantum mechanical transition probability from state \mathbf{k} to state \mathbf{k}' is given by the Fermi golden rule:

$$W_{\mathbf{k}\mathbf{k}'} = \frac{2\pi}{\hbar} n_i \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}) |\langle \mathbf{k}' | U | \mathbf{k} \rangle|^2, \quad (24.4.3)$$

where U is not simply the bare Coulomb potential of impurity ion: the screening effect of the other electrons are also incorporated in it. We shall discuss this in more detail at the end of the section. The matrix element is calculated between Bloch states:

$$\langle \mathbf{k}' | U | \mathbf{k} \rangle = \int d\mathbf{r} \psi_{n\mathbf{k}'}^*(\mathbf{r}) U(\mathbf{r}) \psi_{n\mathbf{k}}(\mathbf{r}). \quad (24.4.4)$$

Because of the random distribution of the impurities, the electrons scattered incoherently by different impurities do not interfere. That is why the transition probability is proportional to the number of scatterers.

³ A. MATTHIESSEN, 1864.

Since scattering by rigid impurities is elastic, the approach of Section 24.2.1 for the treatment of elastic scattering can be applied, and a relaxation time can be introduced through (24.3.13). This expression is further simplified for isotropic Fermi surfaces. Since the velocity $\mathbf{v}_{\mathbf{k}}$ is then parallel to \mathbf{k} , it is natural to assume that $\chi(\mathbf{k})$, the quantity characterizing the departure from equilibrium – which must be proportional to the electric field – can be written as

$$\chi(\mathbf{k}) = a(\varepsilon_{\mathbf{k}})\mathbf{k} \cdot \mathbf{E}. \quad (24.4.5)$$

Substituting this into the formula for the relaxation time, and making use of the elastic character of the scattering, we have

$$\frac{1}{\tau(\mathbf{k})} = \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}\mathbf{k}'} \left(1 - \frac{\mathbf{E} \cdot \mathbf{k}'}{\mathbf{E} \cdot \mathbf{k}} \right). \quad (24.4.6)$$

Let us now separate \mathbf{k}' into components that are parallel and perpendicular to \mathbf{k} . As the two vectors are of the same length,

$$\mathbf{k}' = \mathbf{k}'_{\perp} + (\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')\mathbf{k} = \mathbf{k}'_{\perp} + \cos \theta \mathbf{k}, \quad (24.4.7)$$

where $\hat{\mathbf{k}}$ ($\hat{\mathbf{k}}'$) is the unit vector in the direction \mathbf{k} (\mathbf{k}'), and θ is the angle between \mathbf{k} and \mathbf{k}' . Since only those scattering processes for which both \mathbf{k} and \mathbf{k}' are essentially on the Fermi surface give important contributions, $W_{\mathbf{k}\mathbf{k}'}$ depends only on θ , and is independent of the perpendicular component. The part of $(1 - \mathbf{E} \cdot \mathbf{k}' / \mathbf{E} \cdot \mathbf{k})$ that contains \mathbf{k}'_{\perp} gives vanishing contribution after integration over the azimuthal angle φ , and so the relaxation time is given by

$$\frac{1}{\tau(\mathbf{k})} = \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}\mathbf{k}'} (1 - \cos \theta). \quad (24.4.8)$$

As has already been mentioned, the relaxation time used for the calculation of the electrical conductivity is not the same as the lifetime of an electron of wave vector \mathbf{k} obtained using simple quantum mechanical considerations, which is

$$\frac{1}{\tau(\mathbf{k})} = \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}\mathbf{k}'} . \quad (24.4.9)$$

In this formula each process that scatters the electron of wave vector \mathbf{k} into another state is weighted by its proper transition probability. However, when the resistivity – i.e., the decay of the current – is considered, other factors have to be taken into account as well. Those processes in which the wave vector changes little hardly reduce the current. The effect is the strongest when the electron of wave vector \mathbf{k} is scattered into the state $-\mathbf{k}$, that is, in backscattering. The factor $1 - \cos \theta$ in the transport relaxation time comes precisely from the different weights of forward and backward scattering.

Since the relaxation time was found to be temperature independent, impurity scattering gives a temperature-independent contribution to the resistivity.

Figure 24.5 shows the low-temperature resistivity for two copper samples of different degrees of purity. At very low temperatures all other scattering processes are frozen out, and impurities cause a finite *residual resistivity*, which depends sensitively on the purity of the sample. The ratio of this quantity to the room-temperature resistivity can be used to characterize the purity of the sample.

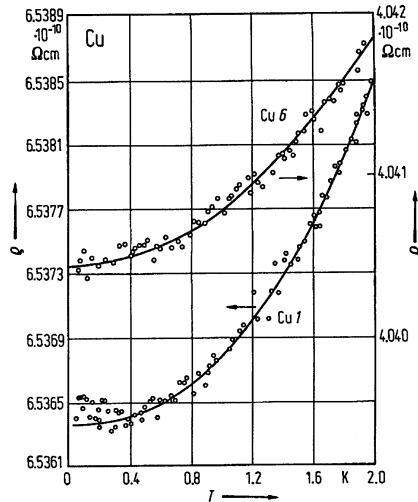


Fig. 24.5. Low-temperature resistivity in two copper samples of different purity [Reprinted with permission from M. Khoshenevisan et al., *Phys. Rev. B* **19**, 3873 (1979). ©1979 by the American Physical Society]

To evaluate the order of magnitude of this resistivity contribution, assumptions have to be made about the strength of the interaction. The simplest option is to assume that the impurity ion has a certain charge, and conduction electrons are scattered by this long-range potential via the Coulomb interaction. We shall see later that far from the impurity conduction electrons screen the charge of the impurity ion, therefore instead of the long-range Coulomb interaction electrons feel a short-range scattering potential. The results obtained in this modified picture for the transport relaxation time and resistivity due to impurities are in agreement with measurement data.

24.4.2 Contribution of Electron–Phonon Scattering to the Resistivity

To determine the contribution of the electron–phonon interaction to the resistivity, the transport equation needs to be solved simultaneously for the electron and phonon systems. In the equation for the electrons the form (24.2.38) of the collision integral has to be used. By making the approximation that, for

the purpose of determining the electron distribution, the system of phonons is in thermal equilibrium ($\phi_\lambda(\mathbf{q}) = 0$), the collision term takes the form

$$\begin{aligned} \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = & -\frac{1}{V} \sum_{\mathbf{q}\lambda} I_{\mathbf{k},\mathbf{q},\lambda} f_0(\mathbf{k}) [1 - f_0(\mathbf{k} + \mathbf{q})] [\chi(\mathbf{k}) - \chi(\mathbf{k} + \mathbf{q})] \\ & \times \{ g_\lambda^0(\mathbf{q}) \delta(\varepsilon_{\mathbf{k}} + \hbar\omega_\lambda(\mathbf{q}) - \varepsilon_{\mathbf{k}+\mathbf{q}}) \\ & + [1 + g_\lambda^0(\mathbf{q})] \delta(\varepsilon_{\mathbf{k}} - \hbar\omega_\lambda(\mathbf{q}) - \varepsilon_{\mathbf{k}+\mathbf{q}}) \}. \end{aligned} \quad (24.4.10)$$

Before deriving an approximately valid formula, we shall analyze two limiting cases, in which the temperature dependence of the resistivity can be simply determined from the number of phonons participating in the collisions and the conservation of energy and momentum.

At temperature T , the electrons in the region of width $k_B T$ around the Fermi energy can participate in collision. At temperatures higher than the characteristic Debye temperature of the phonon spectrum the energy of the phonons is smaller than the thermal energy, therefore the phonon-absorption or -emission processes are quasielastic from the viewpoint of electrons. If the phonon energy may be neglected in the energy-conservation delta function then the two terms in the previous collision integral can be combined. The arising formula is similar to the result obtained in the relaxation-time approximation, however, an additional factor $1 + 2g_\lambda^0(\mathbf{q})$ appears, indicating the presence of phonons. As mentioned before, if it were not for this factor, the relaxation time would be temperature independent. However, the occupation function of phonons is proportional to the temperature in the $T \gg \Theta_D$ region,

$$g_\lambda^0(\mathbf{q}) = \frac{1}{\exp(\beta\hbar\omega_\lambda(\mathbf{q})) - 1} \approx \frac{k_B T}{\hbar\omega_\lambda(\mathbf{q})}, \quad (24.4.11)$$

and thus the inverse relaxation time and the resistivity are both proportional to it, too:

$$\varrho \sim T, \quad \text{if} \quad T \gg \Theta_D. \quad (24.4.12)$$

This result can be interpreted alternatively. The relaxation time contains a certain average of the square of the matrix element of the electron-phonon interaction. Since the matrix element is proportional to the displacement of the ions, $1/\tau$ contains the mean square displacement. It was shown in (12.3.12) that at high temperatures $\langle \mathbf{u}^2 \rangle \sim T$, so the resistivity increases in direct proportion to the temperature.

The situation is more complicated at low temperatures. Even though scattering is quasielastic, the number of electrons and phonons participating in the scattering need to be estimated more accurately: in addition to energy and momentum conservation, the wave-number dependence of the matrix element as well as the asymmetry between the contributions of forward- and backward-scattering processes also have to be taken into account.

Assuming that a single phonon is created or annihilated in the collision,

$$\varepsilon_{\mathbf{k} \pm \mathbf{q}} = \varepsilon_{\mathbf{k}} \pm \hbar\omega_{\lambda}(\mathbf{q}). \quad (24.4.13)$$

If the conservation of energy were considered alone, upon the absorption of a sufficiently energetic phonon an electron sitting relatively deep below the Fermi energy could also be scattered to an empty state above the Fermi level. In reality, however, only energy transfers of order $k_{\text{B}}T$ occur: only those phonons are likely to participate in absorption for which $\hbar\omega_{\lambda}(\mathbf{q}) \leq k_{\text{B}}T$ because only these phonons are excited thermally in sufficient numbers. This implies that only acoustic phonons are relevant, and their wave numbers must satisfy the condition $q \leq k_{\text{B}}T/\hbar c_{\text{s}}$.

The same bound applies to phonon emission. Once a thermally excited electron has emitted a phonon and transferred a part of its energy to the lattice, it has to occupy an initially empty state. Thus both the initial and final states of the electron must be close to the Fermi energy, inside a region that is a few times $k_{\text{B}}T$ wide. Hence the energy loss must be of the same order of magnitude or smaller. This change in the energy is small compared to the energy of the electrons, which is on the order of the Fermi energy, therefore these processes may be called quasielastic.

Now consider the collision integral for wave vectors \mathbf{k} that are close to the Fermi surface. It follows from our previous considerations that substantial contributions come only from those scattering processes for which $\mathbf{k} + \mathbf{q}$ is inside the sphere of radius $k_{\text{B}}T/\hbar c_{\text{s}}$ centered at \mathbf{k} . Energy conservation imposes another constraint, so the wave vectors of phonons participating in scattering lie on a two-dimensional surface inside the sphere. Thus in the sum over the wave vector \mathbf{q} the phase-space restriction gives a factor that is proportional to T^2 .

Another factor comes from the strength of the scattering. According to (24.2.30), the transition probability $W_{\mathbf{k};\mathbf{k}',\mathbf{q},\lambda}$ in the collision integral contains the square of the matrix element of the electron–phonon interaction. As mentioned above, only acoustic phonons need to be taken into account at low temperatures. For acoustic phonons the matrix element of the electron–phonon interaction is proportional to \sqrt{q} . According to the previous dimensional consideration, the factor q coming from the square of the matrix element brings in an additional factor of T .

Altogether, this would mean that the inverse relaxation time due to the electron–phonon interaction is proportional to T^3 – which would lead to $\varrho \sim T^3$ in the $T \ll \Theta_{\text{D}}$ region. However, just like for impurity scattering, a factor $1 - \chi(\mathbf{k}')/\chi(\mathbf{k})$ appears in the collision integral for electron–phonon scattering. At low temperatures, where electron–phonon scattering is quasielastic, this factor can be rewritten as $1 - \cos\theta$. Owing to this factor, forward and small-angle scattering contribute much less to the effective collision rate than large-angle and backward scattering. Since the electron has to be close to the Fermi surface both in the initial and final states, and at low temperatures the wavelength of phonons participating in these scattering processes is much smaller than the Fermi wave number, small-angle scattering dominates, for which

$$1 - \cos \theta = 2 \sin^2(\theta/2) \approx \frac{1}{2} (q/k_F)^2. \quad (24.4.14)$$

This is illustrated in Fig. 24.6.

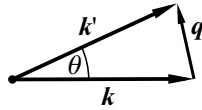


Fig. 24.6. Electron and phonon wave vectors in small-angle quasielastic scattering

According to our previous dimensional considerations, this q^2 term gives an additional factor T^2 to the collision integral, and thus

$$\varrho \sim T^5. \quad (24.4.15)$$

This T^5 dependence becomes modified if the Fermi surface approaches the zone boundary, and thus umklapp scattering become important.

Calculations are very tedious in the region between the two limiting cases. However, a good interpolation formula is offered by the partly empirical *Bloch–Grüneisen relation*:⁴

$$\varrho(T) = K(T/\Theta_D)^5 J_5(\Theta_D/T), \quad (24.4.16)$$

where K is a constant, which will not be specified here, and

$$J_5(x) = \int_0^x \frac{e^\xi \xi^5 d\xi}{(e^\xi - 1)^2} = 5 \int_0^x \frac{\xi^4 d\xi}{e^\xi - 1} - \frac{x^5}{e^x - 1}. \quad (24.4.17)$$

This integral lends itself to simple evaluation in two limits:

$$J_5(x) = \begin{cases} \frac{1}{4}x^4 - \frac{1}{72}x^6 + \dots & x \ll 1, \\ 5! \sum_{k=1}^{\infty} \frac{1}{k^5} = 5!\zeta(5) = 124.43 & x \gg 1. \end{cases} \quad (24.4.18)$$

At low temperatures ($\Theta_D/T \gg 1$), $J_5(\Theta_D/T)$ is constant, so the resistivity is proportional to the fifth power of the temperature. Likewise, at high temperatures ($\Theta_D/T \ll 1$), $J_5(\Theta_D/T)$ is proportional to $(1/T)^4$, so the resistivity is proportional to the temperature. In both limits the previous results are recovered, and the interpolation formula provides a good approximation for the resistivity of simple metals in the intermediate region, too. This is shown in Fig. 24.7.

At very low temperatures electron–electron scattering has to be taken into account, too. It can be demonstrated that the requirements of energy

⁴ F. BLOCH, 1930; E. GRÜNEISEN, 1933.

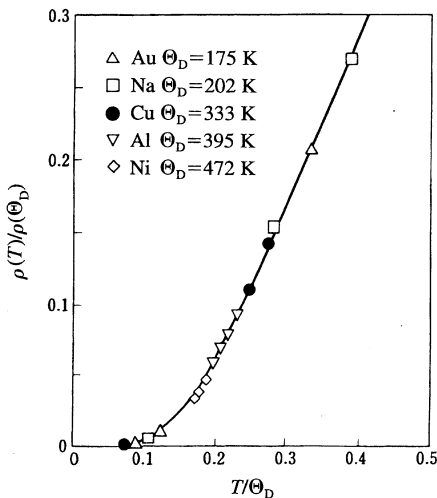


Fig. 24.7. The resistivity of some simple metals scaled by the resistivity at the Debye temperature, as a function of T/Θ_D . The solid line is the prediction of the Bloch–Grüneisen formula [F. J. Blatt, *Physics of Electronic Conduction in Solids*, McGraw-Hill Book Co., New York (1968)]

and momentum conservation can be satisfied simultaneously only by umklapp processes. After some algebra, the resistivity is found to be proportional to the square of the temperature:

$$\varrho_{\text{el-el}} \sim \left(\frac{k_B T}{\varepsilon_F} \right)^2. \quad (24.4.19)$$

In alkali metals $\tau_{\text{el-ph}}$ and $\tau_{\text{el-el}}$ are comparable at a few kelvins (around 4 K for sodium), however a relatively low concentration of impurities gives rise to a similar relaxation time. The contributions of individual processes are difficult to separate.

The situation is different in transition metals. The electric current is dominantly carried by s -electrons, nevertheless the interaction with d -electrons, whose density of states is high, can give an important contribution to the resistivity. In some transition metals (Mn, Fe, Co, Ni, Pd, Pt, W, and Nb) the temperature dependence of the resistivity below 10 K is fairly well approximated by a quadratic fit, as shown in Fig. 24.8. It should be noted that other scattering processes can also lead to such a temperature dependence in magnetic materials – but the majority of the materials listed above are not magnetic.

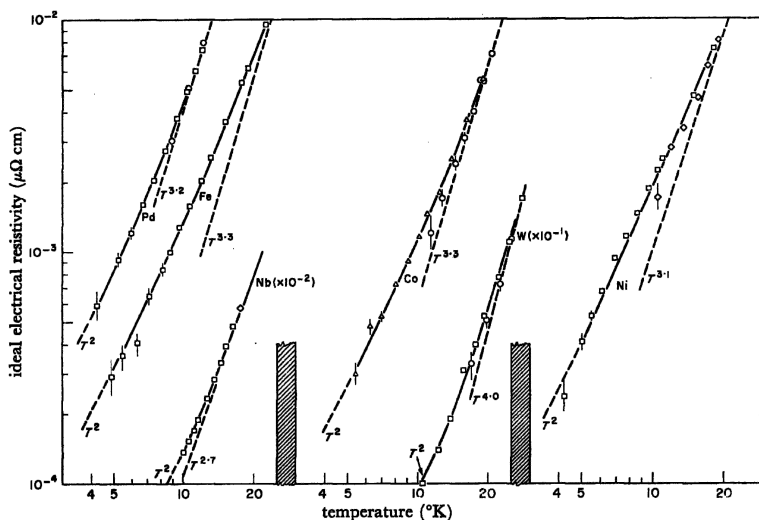


Fig. 24.8. Temperature dependence of resistivity for some transition metals (Pd, Fe, Nb, Co, W, Ni) at temperatures below 20 K [G. K. White and S. B. Woods, *Philosophical Transactions of the Royal Society*, **251** A, 273 (1959)]

24.4.3 Scattering by Magnetic Impurities and the Kondo Effect

The ubiquitous impurities in metals give a temperature-independent contribution to the resistivity, the so-called residual resistivity (page 389). However, strong temperature dependence was observed in several low-temperature experiments: the resistivity attained a minimum at a few kelvins, and then started to grow with decreasing temperature as $\log T$, see Fig. 24.9.

Since measurements indicated the possibility that the effect might be due to the presence of magnetic impurities, J. KONDO (1964) justified by theoretical calculations that scattering by such impurities indeed gives rise to an increase in the resistivity with decreasing temperature. Earlier calculations of impurity scattering were based on a spin-independent scattering potential. However, when magnetic impurities (Mn, Cr, Fe, etc.) are introduced into a nonmagnetic metal (Cu, Ag, Au, Al, etc.), spin-flip processes become possible: the spin of the scattered electron and the spin of the magnetic impurity are flipped simultaneously, while the component of the total spin along the quantization axis is conserved. This opens a new scattering channel. The interaction of the impurity with conduction electrons is described in terms of the so-called s - d interaction, in which the spin \mathbf{S}_i of the impurity located at \mathbf{R}_i – which is an internal degree of freedom of the impurity – interacts with the local spin density of the conduction electrons. When electrons are represented by field operators or by creation and annihilation operators of free-electron states (as the periodic potential of the lattice is neglected in the present calculation), the interaction Hamiltonian takes the form

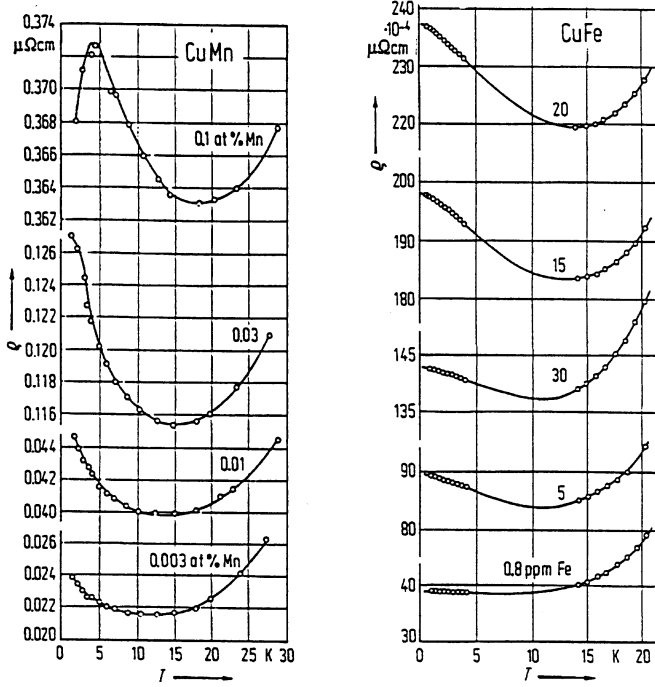


Fig. 24.9. Temperature dependence of resistivity in copper containing a small concentration of magnetic impurities (manganese and iron) [G. Grüner, *Advances in Physics* **23**, 941 (1974), and B. Knook, *Thesis*, Leiden (1962)]

$$\begin{aligned}
 \mathcal{H}_{s-d} &= -J \sum_{i\alpha\beta} \int \hat{\psi}_{\alpha}^{\dagger}(\mathbf{r}) \boldsymbol{\sigma}_{\alpha\beta} \hat{\psi}_{\beta}(\mathbf{r}) \cdot \mathbf{S}_i \delta(\mathbf{r} - \mathbf{R}_i) d\mathbf{r} \\
 &= -\frac{J}{V} \sum_i \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_i} c_{\mathbf{k}'\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k}\beta} \cdot \mathbf{S}_i.
 \end{aligned} \tag{24.4.20}$$

Since the flip of the impurity spin is accompanied by the flip of an electron spin, separate equations have to be written down for the distribution function of spin-up and spin-down electrons. The collision term for the former is

$$\begin{aligned}
 \left(\frac{\partial f_{\uparrow}(\mathbf{k})}{\partial t} \right)_{\text{coll}} &= \sum_{\mathbf{k}'} W_{\mathbf{k}\uparrow, \mathbf{k}'\uparrow} \{ f_{\uparrow}(\mathbf{k}') [1 - f_{\uparrow}(\mathbf{k})] - f_{\uparrow}(\mathbf{k}) [1 - f_{\uparrow}(\mathbf{k}')] \} \\
 &\quad + \sum_{\mathbf{k}'} W_{\mathbf{k}\uparrow, \mathbf{k}'\downarrow} \{ f_{\downarrow}(\mathbf{k}') [1 - f_{\uparrow}(\mathbf{k})] - f_{\uparrow}(\mathbf{k}) [1 - f_{\downarrow}(\mathbf{k}')] \}.
 \end{aligned} \tag{24.4.21}$$

The transition probability W_{ab} between states a and b is given by the usual quantum mechanical formula

$$W_{ab} = \frac{2\pi}{\hbar} |\langle a | \mathcal{H}_{\text{s-d}} | b \rangle|^2 \delta(\varepsilon_a - \varepsilon_b). \quad (24.4.22)$$

For spin-conserving scattering, the matrix element is

$$\langle \mathbf{k}' \uparrow | \mathcal{H}_{\text{s-d}} | \mathbf{k} \uparrow \rangle = -\frac{J}{V} S^z. \quad (24.4.23)$$

By determining the other matrix elements it is relatively straightforward to show that the residual resistivity is temperature independent in this case, too, just like for nonmagnetic impurities. KONDO's important observation was that, despite the weakness of the coupling, the Born approximation does not provide a satisfactory treatment of the scattering: higher-order corrections need to be taken into account as well.

A better approximation can be obtained for the transition probability by replacing the matrix element of the interaction Hamiltonian by the matrix element of the scattering matrix T in (24.4.22). When the eigenstates $|a\rangle$ and energy eigenvalues ε_a of the unperturbed system are known, the transition probability from $|a\rangle$ to $|b\rangle$ due to the interaction is

$$W_{ab} = \frac{2\pi}{\hbar} |\langle a | T | b \rangle|^2 \delta(\varepsilon_a - \varepsilon_b), \quad (24.4.24)$$

where the matrix elements of T can be expressed in terms of those of the interaction Hamiltonian \mathcal{H}_{int} as

$$\langle a | T | b \rangle = \langle a | \mathcal{H}_{\text{int}} | b \rangle + \sum_c \frac{\langle a | \mathcal{H}_{\text{int}} | c \rangle \langle c | \mathcal{H}_{\text{int}} | b \rangle}{\varepsilon_a - \varepsilon_c} + \dots \quad (24.4.25)$$

Up to the third order in the coupling constant,

$$\begin{aligned} W_{ab} = \frac{2\pi}{\hbar} \bigg\{ & \langle a | \mathcal{H}_{\text{s-d}} | b \rangle \langle b | \mathcal{H}_{\text{s-d}} | a \rangle \\ & + \sum_c \left[\frac{\langle a | \mathcal{H}_{\text{s-d}} | c \rangle \langle c | \mathcal{H}_{\text{s-d}} | b \rangle \langle b | \mathcal{H}_{\text{s-d}} | a \rangle}{\varepsilon_a - \varepsilon_c} + \text{c.c.} \right] + \dots \bigg\} \delta(\varepsilon_a - \varepsilon_b). \end{aligned} \quad (24.4.26)$$

First consider the scattering $\mathbf{k} \uparrow \rightarrow \mathbf{k}' \uparrow$. As shown in Fig. 24.10, two processes are possible in second order. One option is that the electron of quantum numbers $\mathbf{k} \uparrow$ is first scattered into an intermediate state

$$|c\rangle = |\mathbf{k}''\sigma\rangle = c_{\mathbf{k}''\sigma}^\dagger |FS\rangle, \quad (24.4.27)$$

and then, in a second event, the electron of quantum numbers $\mathbf{k}''\sigma$ is scattered to the final state $\mathbf{k}' \uparrow$.

The other option is that the first interaction leaves the electron of quantum numbers $\mathbf{k} \uparrow$ in its initial state, and the impurity spin interacts with the Fermi sea to create an electron-hole pair. The intermediate state thus contains the electron $\mathbf{k} \uparrow$ as well as an electron-hole pair:



Fig. 24.10. Second-order processes of the s - d interaction. Time flows from left to right. The electron propagating backward in time corresponds to a hole

$$|c\rangle = |\mathbf{k}\uparrow, \mathbf{k}'\uparrow, \mathbf{k}''\sigma\rangle = c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\uparrow}^\dagger c_{\mathbf{k}''\sigma} |\text{FS}\rangle. \quad (24.4.28)$$

The hole of quantum numbers $\mathbf{k}''\sigma$ is filled by the hitherto unperturbed incoming electron $\mathbf{k}\uparrow$ in the second interaction, while the electron of the created electron-hole pair survives in the final state. In the previous formulas only the states of the electrons are indicated, those of the impurity spin are not. We shall need to pay attention to this.

In order that these processes can take place, the state $\mathbf{k}''\sigma$ has to be initially empty in the first, and occupied in the second case. The second-order correction to the T matrix is

$$\begin{aligned} T^{(2)} = & \sum_{\mathbf{k}''\sigma} \frac{\langle \mathbf{k}\uparrow | \mathcal{H}_{s-d} | \mathbf{k}''\sigma \rangle \langle \mathbf{k}''\sigma | \mathcal{H}_{s-d} | \mathbf{k}'\uparrow \rangle}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}''}} (1 - f_0(\mathbf{k}'')) \\ & + \sum_{\mathbf{k}''\sigma} \frac{\langle \mathbf{k}\uparrow | \mathcal{H}_{s-d} | \mathbf{k}\uparrow, \mathbf{k}'\uparrow, \mathbf{k}''\sigma \rangle \langle \mathbf{k}\uparrow, \mathbf{k}'\uparrow, \mathbf{k}''\sigma | \mathcal{H}_{s-d} | \mathbf{k}'\uparrow \rangle}{\varepsilon_{\mathbf{k}} - (\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}''})} f_0(\mathbf{k}''). \end{aligned} \quad (24.4.29)$$

If the z component of the impurity spin is left unchanged by the scattering, the combined contribution of the two channels is

$$\begin{aligned} & \left(-\frac{J}{V}\right)^2 \sum_{\mathbf{k}''} (S^z)^2 \left(\frac{1 - f_0(\mathbf{k}'')}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}''}} - \frac{f_0(\mathbf{k}'')}{\varepsilon_{\mathbf{k}''} - \varepsilon_{\mathbf{k}'}} \right) \\ & = \left(-\frac{J}{V}\right)^2 (S^z)^2 \sum_{\mathbf{k}''} \frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}''}}. \end{aligned} \quad (24.4.30)$$

The negative sign of the second term on the left-hand side is the consequence of the Fermi-Dirac statistics. Assuming that the density of states is symmetric about the Fermi energy, the integral vanishes for the electrons on the Fermi surface, and is negligible in its vicinity. The contribution of scattering by a rigid, nonrotating spin – just like that of potential scattering – is of no interest.

On the other hand, if the spin is flipped in the intermediate state, then an electron of quantum numbers $\mathbf{k}''\downarrow$ appears in the first process, and the impurity spin goes over from the initial state $S^z = M$ to $S^z = M + 1$. The contribution of this process is

$$\left(-\frac{J}{V}\right)^2 \sum_{\mathbf{k}''} [S(S+1) - M(M+1)] \frac{1 - f_0(\mathbf{k}'')}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}''}}. \quad (24.4.31)$$

In the other channel, where the electron-hole pair is composed of a spin-up electron and a spin-down hole, the impurity spin has to flip down, to the state $S^z = M - 1$. The contribution of this process is therefore

$$- \left(-\frac{J}{V} \right)^2 \sum_{\mathbf{k}''} [S(S+1) - M(M-1)] \frac{f_0(\mathbf{k}'')}{\varepsilon_{\mathbf{k}} - (\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}'})}. \quad (24.4.32)$$

Since $\varepsilon_{\mathbf{k}} = \varepsilon_{\mathbf{k}'}$ on account of the conservation of energy, the combined contribution is

$$\left(-\frac{J}{V} \right)^2 \sum_{\mathbf{k}''} \left\{ [S(S+1) - M^2] \frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}''}} - M \frac{1 - 2f_0(\mathbf{k}'')}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}''}} \right\}. \quad (24.4.33)$$

The first term is negligible once again, however, the second term is no longer small: it even diverges logarithmically when $\varepsilon_{\mathbf{k}} \rightarrow \varepsilon_F$ and $T \rightarrow 0$.

Using this form for the second-order correction to the T matrix in J , the transition probability can be determined up to third order in J . By summing over the possible spin orientations,

$$W(\mathbf{k} \uparrow \rightarrow \mathbf{k}' \uparrow) = n_i \frac{2\pi J^2 S(S+1)}{3\hbar} [1 + 4Jg(\varepsilon_{\mathbf{k}})] \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}), \quad (24.4.34)$$

where n_i is the concentration of magnetic impurities, and the singular function in the third-order correction is

$$g(\varepsilon_{\mathbf{k}}) = \frac{1}{V} \sum_{\mathbf{k}''} \frac{f_0(\mathbf{k}'')}{\varepsilon_{\mathbf{k}''} - \varepsilon_{\mathbf{k}}}. \quad (24.4.35)$$

To evaluate this sum, we assume a constant density of states. This is a good approximation for electrons close to the Fermi surface, from where the singular contribution to the corresponding integral comes. This gives

$$g(\varepsilon_{\mathbf{k}}) \sim \begin{cases} \ln(k_B T / \varepsilon_F), & \text{if } \varepsilon_{\mathbf{k}} < k_B T, \\ \ln(\varepsilon_{\mathbf{k}} / \varepsilon_F), & \text{if } \varepsilon_{\mathbf{k}} > k_B T. \end{cases} \quad (24.4.36)$$

Repeating the calculation for the spin-flip scattering $\mathbf{k} \uparrow \rightarrow \mathbf{k}' \downarrow$,

$$W(\mathbf{k} \uparrow \rightarrow \mathbf{k}' \downarrow) = n_i \frac{4\pi J^2 S(S+1)}{3\hbar} [1 + 4Jg(\varepsilon_{\mathbf{k}})] \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}). \quad (24.4.37)$$

By substituting these formulas into the collision integral, we can define a relaxation time in the customary way. The result is

$$\frac{1}{\tau} = n_i \frac{3\pi J^2 S(S+1)z}{2\hbar\varepsilon_F} [1 + 4Jg(\varepsilon_{\mathbf{k}})], \quad (24.4.38)$$

where z is the number of conduction electrons per atom.

Using this energy- or temperature-dependent relaxation time in the Boltzmann equation,

$$\varrho = \varrho_0 + A \ln T \quad (24.4.39)$$

is obtained for the resistivity after some algebra. Here ϱ_0 is the resistivity of the pure sample.

Using this formula, a good fit can be obtained for the experimental results in the vicinity of the resistivity minimum. However, because of the logarithmic temperature dependence, the question immediately arises: What happens at lower temperatures? It is straightforward to show that the higher orders of the perturbation expansion give even more singular contributions, and thus perturbation theory is unable to provide a satisfactory treatment of the problem. This made the Kondo problem one of the most intensely studied problems of solid-state physics in the past decades. We shall return to it in Chapter 35 on strongly correlated electron systems.

24.4.4 Electronic Contribution to Thermal Conductivity

As was shown on page 380, the Wiedemann–Franz law, which is based on experimental findings, applies to Bloch electrons as well in the relaxation-time approximation. Therefore the electronic contribution to thermal conductivity could be determined naively but most straightforwardly using this law. Thus, the product of the thermal conductivity and the resistivity is expected to be proportional to the temperature, with a universal constant of proportionality, the Lorenz number given in (16.3.48). Using our previous results for the temperature dependence of the resistivity,

$$\varrho \sim \begin{cases} \text{const.}, & \text{if } T \rightarrow 0, \\ T^5, & \text{if } T < \Theta_D, \\ T, & \text{if } T > \Theta_D, \end{cases} \quad (24.4.40)$$

the thermal conductivity should then behave as

$$\lambda \sim \begin{cases} T, & \text{if } T \rightarrow 0, \\ T^{-4}, & \text{if } T < \Theta_D, \\ \text{const.}, & \text{if } T > \Theta_D \end{cases} \quad (24.4.41)$$

in the three temperature ranges of interest. Typical experimental results for metals are shown in Fig. 24.11.

The thermal conductivity is proportional to the temperature at low temperatures, as expected, but the constant of proportionality depends strongly on the purity of the sample. At high temperatures, too, the theoretical prediction is in agreement with the experimental findings: λ tends to a constant. However, the Wiedemann–Franz law fails in the intermediate temperature range: the thermal conductivity is proportional to $1/T^2$ rather than $1/T^4$

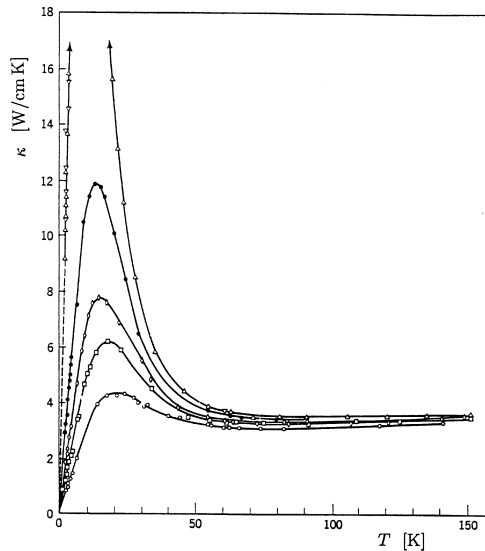


Fig. 24.11. Temperature dependence of the thermal conductivity for gold samples of different purity [J. Olsen, *Electron Transport in Metals*, Interscience Publishers, Inc., New York (1962)]

here. The experimentally observed tendency T^{-2} can be reproduced in theoretical calculations by omitting the factor $1 - \cos \theta$ in the relaxation rate. This factor played an essential role in the determination of the resistivity but seems to be unimportant in heat-conduction phenomena. This can be understood intuitively, as electron-phonon scattering cannot be considered elastic in this region, and thus the relaxation-time approximation is inapplicable. While small-angle inelastic scattering by low-momentum phonons gives a very small contribution to the decay of the electric current, the same processes contribute appreciably to the decay of the heat current, as electrons lose energy in such processes.

24.4.5 Phonon Contribution to Thermal Conductivity

Up to now we have considered only electrons as a vehicle of heat conduction. However, phonons can also contribute to thermal conductivity in solids. Note that when only normal processes are considered, in which energy and momentum are conserved simultaneously, the heat current cannot decay. If it were not for umklapp processes, solids would be perfect heat conductors.

The heat current carried by phonons can be simply written as

$$\mathbf{j}_Q = \sum_{\lambda} \int \frac{d\mathbf{q}}{(2\pi)^3} \hbar \omega_{\lambda}(\mathbf{q}) \mathbf{v}_{\lambda}(\mathbf{q}) g(\mathbf{q}), \quad (24.4.42)$$

where $\mathbf{v}_\lambda(\mathbf{q})$ is the group velocity of phonons. The Boltzmann equation governing the stationary distribution function of phonons in the presence of a temperature gradient was given in (24.2.28). Applying the relaxation-time approximation, its solution is

$$g_\lambda(\mathbf{q}) = g_\lambda^0(\mathbf{q}) - \tau(\mathbf{q}) \frac{\partial g_\lambda^0(\mathbf{q})}{\partial T} \mathbf{v}_\lambda(\mathbf{q}) \cdot \nabla T. \quad (24.4.43)$$

Substituting this into the current formula,

$$\mathbf{j}_Q = -\nabla T \sum_\lambda \int \frac{d\mathbf{q}}{(2\pi)^3} \hbar \omega_\lambda(\mathbf{q}) \mathbf{v}_\lambda(\mathbf{q}) \circ \mathbf{v}_\lambda(\mathbf{q}) \tau(\mathbf{q}) \frac{\partial g_\lambda^0(\mathbf{q})}{\partial T} \quad (24.4.44)$$

is obtained, and thus the thermal conductivity is

$$\lambda = \frac{1}{3} \sum_\lambda \int \frac{d\mathbf{q}}{(2\pi)^3} \hbar \omega_\lambda(\mathbf{q}) v_\lambda(\mathbf{q}) \Lambda_\lambda(\mathbf{q}) \frac{\partial g_\lambda^0(\mathbf{q})}{\partial T} \quad (24.4.45)$$

in the isotropic case, where $\Lambda_\lambda(\mathbf{q}) = v_\lambda(\mathbf{q}) \tau(\mathbf{q})$ is the mean free path. In terms of $c_\lambda(\mathbf{q})$, the heat capacity per mode, this can be rewritten as

$$\lambda = \frac{1}{3} \sum_\lambda \int \frac{d\mathbf{q}}{(2\pi)^3} c_\lambda(\mathbf{q}) v_\lambda(\mathbf{q}) \Lambda_\lambda(\mathbf{q}). \quad (24.4.46)$$

Note that this is the generalization of (12.4.20),

$$\lambda = \frac{1}{3} c_V \bar{v} \Lambda, \quad (24.4.47)$$

a well-known formula of the kinetic theory of gases.

At temperatures well above the Debye temperature the mean free path of phonons is inversely proportional to the temperature, $\Lambda \sim 1/T$, and thus the thermal conductivity also decreases with increasing temperature:

$$\lambda \sim 1/T. \quad (24.4.48)$$

At low temperatures umklapp processes freeze out. The strength of those processes in which two phonons (\mathbf{q} and \mathbf{q}') merge into one (\mathbf{q}'') is proportional to the occupation of the initial states, given by

$$g_\lambda(\mathbf{q}) g_{\lambda'}(\mathbf{q}') \sim \exp\left(-\frac{\hbar \omega_\lambda(\mathbf{q})}{k_B T}\right) \exp\left(-\frac{\hbar \omega_{\lambda'}(\mathbf{q}')}{k_B T}\right). \quad (24.4.49)$$

Because of the conservation of energy,

$$g_\lambda(\mathbf{q}) g_{\lambda'}(\mathbf{q}') \sim \exp\left(-\frac{\hbar \omega_{\lambda''}(\mathbf{q}'')}{k_B T}\right) \sim \exp\left(-\frac{\Theta_D}{T}\right) \quad (24.4.50)$$

for phonon states close to the zone boundary at low temperatures. The temperature dependence of the thermal conductivity is then

$$\lambda \sim T^n \exp\left(\frac{\Theta_D}{T}\right), \quad (24.4.51)$$

where the exponent n cannot be determined from our previous considerations. At low temperatures, where umklapp processes become less and less probable, the thermal conductivity would increase beyond bounds in the $T \rightarrow 0$ limit. However, when the mean free path becomes comparable to the size D of the sample, this tendency is reversed, and

$$\lambda \sim T^3 D, \quad (24.4.52)$$

where T^3 comes from the phonon specific heat. This can be readily observed in experiments. Phonons may also be scattered because of the different mass of isotopes. The corresponding, observable, contribution is

$$\lambda \sim \frac{M}{\delta M} \frac{1}{T^{1/2}}. \quad (24.4.53)$$

The left-hand side of Fig. 24.12 shows these characteristic ranges of the thermal conductivity vs. temperature graph on a typical curve, while the right-hand side is a log-log plot of the experimental results for sodium fluoride.

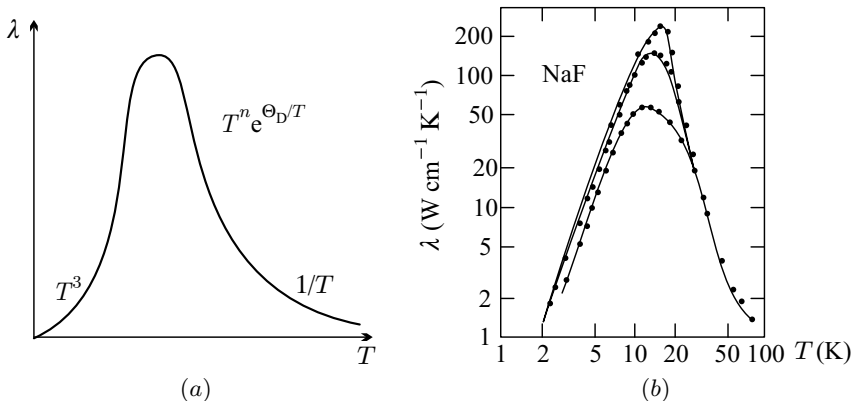


Fig. 24.12. (a) Typical temperature dependence of the thermal conductivity for insulators. (b) The measured thermal conductivity for three differently grown samples of the ionic crystal NaF [Reprinted with permission from H. E. Jackson et al., *Phys. Rev. Lett.* **25**, 26 (1970). ©1970 by the American Physical Society]

24.4.6 Transport Coefficients in Semiconductors

The formulas obtained in the relaxation-time approximation for a gas of free electrons in Chapter 16 will serve as the starting point for our study of transport phenomena in semiconductors. Expressed in terms of K_0 , defined in (16.3.33), the electrical conductivity is

$$\sigma = e^2 \int \frac{d\mathbf{k}}{4\pi^3} \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \tau(\varepsilon_{\mathbf{k}}) \frac{1}{3} v_{\mathbf{k}}^2. \quad (24.4.54)$$

There are two essential differences with metals. Firstly, the classical Maxwell-Boltzmann statistics can be applied instead of quantum statistics; secondly, the contributions of conduction-band electrons and valence-band holes have to be treated separately.

If conduction electrons at the bottom of the conduction band are treated as free particles of effective mass m_n^* , $v_{\mathbf{k}}^2$ can be expressed in terms of the energy, and the \mathbf{k} -sum can be transformed into an energy integral using the density of states. We then have

$$\sigma = \frac{2e^2}{3m_n^*} \int_{\varepsilon_c}^{\infty} \tau(\varepsilon) \left(-\frac{\partial f_0}{\partial \varepsilon} \right) (\varepsilon - \varepsilon_c) \rho_c(\varepsilon) d\varepsilon. \quad (24.4.55)$$

For the density of states we shall use the formula (20.3.1),

$$\rho_c(\varepsilon) = \frac{1}{2\pi^2} \left(\frac{2m_n^*}{\hbar^2} \right)^{3/2} \sqrt{\varepsilon - \varepsilon_c}. \quad (24.4.56)$$

The applicability of classical statistics means that f_0 can be approximated by

$$f_0(\varepsilon) = \frac{1}{e^{(\varepsilon - \mu)/k_B T} + 1} \approx e^{-(\varepsilon - \mu)/k_B T} e^{-(\varepsilon - \varepsilon_c)/k_B T}. \quad (24.4.57)$$

According to (20.3.17) and (20.3.18), the density of excited electrons and the chemical potential are related by

$$n(T) = \frac{1}{4} \left(\frac{2m_n^* k_B T}{\pi \hbar^2} \right)^{3/2} e^{-(\varepsilon_c - \mu)/k_B T}, \quad (24.4.58)$$

and so

$$f_0(\varepsilon) \approx 4n(T) \left(\frac{2m_n^* k_B T}{\pi \hbar^2} \right)^{-3/2} e^{-(\varepsilon - \varepsilon_c)/k_B T}. \quad (24.4.59)$$

Substituting this into the conductivity formula,

$$\sigma = e^2 \frac{4n(T)}{3m_n^* \pi^{1/2}} (k_B T)^{-5/2} \int_{\varepsilon_c}^{\infty} d\varepsilon e^{-(\varepsilon - \varepsilon_c)/k_B T} \tau(\varepsilon) (\varepsilon - \varepsilon_c)^{3/2}. \quad (24.4.60)$$

By introducing the new variable $x = (\varepsilon - \varepsilon_c)/k_B T$,

$$\sigma = e^2 \frac{4n(T)}{3m_n^* \pi^{1/2}} \int_0^{\infty} \tau(\varepsilon) e^{-x} x^{3/2} dx. \quad (24.4.61)$$

Writing the conductivity in the customary Drude form

$$\sigma = \frac{ne^2}{m_n^*} \langle \tau \rangle, \quad (24.4.62)$$

the mean relaxation time is

$$\langle \tau \rangle = \frac{4}{3\pi^{1/2}} \int_0^\infty \tau(\varepsilon) x^{3/2} e^{-x} dx. \quad (24.4.63)$$

This can be rewritten as

$$\langle \tau \rangle = \frac{2}{3k_B T} \frac{\int (\varepsilon - \varepsilon_c) \tau(\varepsilon) e^{-(\varepsilon - \varepsilon_c)/k_B T} \rho(\varepsilon) d\varepsilon}{\int e^{-(\varepsilon - \varepsilon_c)/k_B T} \rho(\varepsilon) d\varepsilon}. \quad (24.4.64)$$

The conductivity of semiconductors is customarily given in terms of the mobility μ defined by $\mathbf{v}_n = -\mu_n \mathbf{E}$. On account of the relationship $\mathbf{j}_n = -en\mathbf{v}_n$ between the current and the drift velocity,

$$\sigma = ne\mu_n, \quad (24.4.65)$$

while the mobility and the relaxation time are related by

$$\mu_n = \frac{e}{m_n^*} \langle \tau \rangle. \quad (24.4.66)$$

Analogous formulas apply to the hole conductivity. The total conductivity is then

$$\sigma = ne\mu_n + pe\mu_p. \quad (24.4.67)$$

The temperature dependence of the conductivity (resistivity) is therefore determined by the number of charge carriers and their mobilities.

At low temperatures impurity scattering is the dominant scattering mechanism in semiconductors, too, however these impurities are usually charged. In Chapter 29 of Volume 3 we shall see that the Coulomb potential of external charges is screened by mobile electrons, and thus the $1/r$ Coulomb potential is replaced by the exponentially screened Yukawa potential:

$$U(r) \propto \frac{e^{-qr}}{r}, \quad (24.4.68)$$

where, owing to the low electron density in semiconductors, the inverse of the screening length can be specified using the classical Debye–Hückel theory of screening: $q_{DH}^2 = n_e e^2 / (\epsilon k_B T)$, where ϵ is the permittivity. When the matrix element in the transition probability is determined using this potential, the transport relaxation time is given by

$$\frac{1}{\tau(\varepsilon)} \sim \varepsilon^{-3/2} \quad (24.4.69)$$

if only the energy dependence of the dominant term is retained. The temperature dependence of the mobility is then

$$\mu \sim \langle \tau \rangle \sim (k_B T)^{3/2}. \quad (24.4.70)$$

The deformation potential offers a particularly well adapted approach to studying the scattering by acoustic phonons. The scattering matrix element leads to an energy- and temperature-dependent relaxation time,

$$\frac{1}{\tau(\varepsilon, T)} \sim \varepsilon^{1/2} k_B T, \quad (24.4.71)$$

which, in conjunction with (24.4.63), gives

$$\mu \sim \langle \tau \rangle \sim (k_B T)^{-3/2}. \quad (24.4.72)$$

Studying the interaction with optical phonons is not so straightforward as the involved processes are not elastic. At low temperatures ($k_B T \ll \hbar \omega_0$) the crucial factor is the number of thermally excited optical phonons,

$$\frac{1}{\tau(\varepsilon)} \sim \frac{1}{e^{\hbar \omega_0 / k_B T} - 1} \sim e^{-\hbar \omega_0 / k_B T}, \quad (24.4.73)$$

and thus

$$\mu \sim \langle \tau \rangle \sim e^{\hbar \omega_0 / k_B T}, \quad (24.4.74)$$

whereas at high temperatures the result is the same as for acoustic phonons:

$$\frac{1}{\tau(\varepsilon)} \sim k_B T \varepsilon^{1/2} \quad \text{and} \quad \mu \sim \langle \tau \rangle \sim T^{-3/2}. \quad (24.4.75)$$

24.5 Quantum Hall Effect

The semiclassical calculation lead to the conclusion that the Hall resistance, which is related to an off-diagonal component of the conductivity tensor, has to be proportional to the magnetic field, whereas ϱ_{xx} has to be practically independent of it. However, in their experiments on silicon-based MOSFETs, VON KLITZING and his coworkers⁵ found that in strong magnetic fields and at low temperatures (at most 1 to 2 kelvins) ϱ_{xy} does not increase proportionally with B but plateaux appear, and the longitudinal resistivity ϱ_{xx} is not constant but oscillates violently and vanishes at the plateaux. Similar behavior is observed when, instead of tuning the magnetic field strength to control which Landau level is filled partially, the gate voltage is changed to modulate the number of charge carriers. This is shown in Fig. 24.13. At or above liquid-helium temperature practically nothing remains of this anomalous behavior.

⁵ K. V. KLITZING, G. DORDA, and M. PEPPER, 1980. See the footnote on page 6 of Volume 1.

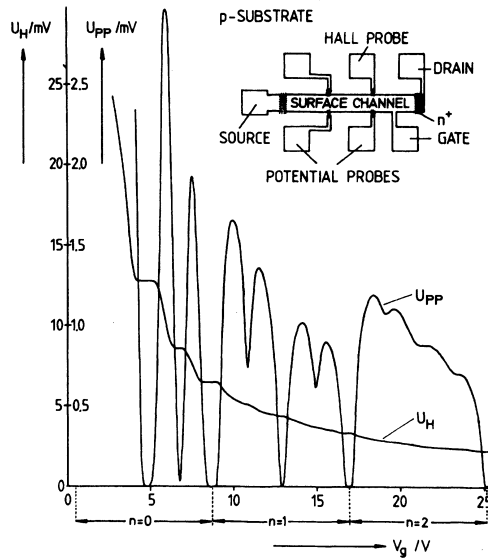


Fig. 24.13. The first experimental results of von Klitzing and coworkers for the quantum Hall effect [Reprinted with permission from *Phys. Rev. Lett.* **45**, 494 (1980). ©1980 by the American Physical Society]

As will be discussed in Chapter 27 on semiconductor devices, an inversion layer may appear at the insulator–semiconductor interface, in which the conduction band is pushed below the chemical potential. The electric field, which is perpendicular to the surface, attracts the electrons into this layer. The thickness of the layer and the number of charge carriers within it can be controlled by the gate voltage V_g . Since the typical width of this layer is 3 to 5 nm, an essentially two dimensional electron gas (2DEG)⁶ appears, and the motion in the perpendicular direction freezes out. As backed up by a multitude of other experiments, the appearance of the plateaux is indeed related to the two-dimensional character of the motion of electrons, and impurities play an important role in it.

Applying the results obtained for the Hall effect to the two-dimensional case, the conductivity tensor is

$$\sigma_{\alpha\beta}(B) = \sigma_0 \begin{pmatrix} \frac{1}{1 + (\omega_c\tau)^2} & \frac{-\omega_c\tau}{1 + (\omega_c\tau)^2} \\ \frac{\omega_c\tau}{1 + (\omega_c\tau)^2} & \frac{1}{1 + (\omega_c\tau)^2} \end{pmatrix}, \quad (24.5.1)$$

where σ_0 is the Drude conductivity. Its inverse is the resistivity tensor,

⁶ The abbreviation 2DES for *two-dimensional electron system* is also commonly used.

$$\varrho_{\alpha\beta}(B) = \varrho_0 \begin{pmatrix} 1 & \omega_c \tau \\ -\omega_c \tau & 1 \end{pmatrix} = \begin{pmatrix} \varrho_0 & B/n_e e \\ -B/n_e e & \varrho_0 \end{pmatrix}. \quad (24.5.2)$$

Apparently, the two-dimensional case does not differ essentially from the previously studied case: in an isotropic system the longitudinal resistivity is independent of the magnetic field, and the Hall resistance increases in direct proportion to the applied field. In contrast, measurements show that the Hall resistance of a doped two-dimensional electron system⁷ features plateaux at

$$\varrho_{xy}^{(\nu)} = \frac{1}{\nu} \frac{h}{e^2}, \quad (24.5.3)$$

where ν is an integer. Therefore the effect is called *integer quantum Hall effect* (IQHE). When $1/\varrho_{xy}$ is plotted against $1/B$, the plateaux are regularly spaced. Moreover, the value of the off-diagonal element of the resistance tensor at the plateaux agrees to a relative accuracy of 10^{-9} with $1/\nu$ times the value $R_K = 25.812\,807\,572\,\text{k}\Omega$, which is calculated from $R_K = h/e^2$. This quantity has since been termed the *von Klitzing constant*. Owing to this extraordinary precision, the quantum Hall effect was adopted in 1990 to establish a new standard for the electrical resistance. By agreement, the conventional value $R_K = 25\,812.807\,\Omega$ was chosen for the Hall resistance of the plateau of label $\nu = 1$.

The xx component of the resistivity tensor, ϱ_{xx} , exhibits strong Shubnikov-de Haas oscillations, and drops to zero wherever the Hall resistance has a plateau. Since

$$\sigma_{xx} = \frac{\varrho_{xx}}{\varrho_{xx}^2 + \varrho_{xy}^2}, \quad \sigma_{xy} = -\frac{\varrho_{xy}}{\varrho_{xx}^2 + \varrho_{xy}^2}, \quad (24.5.4)$$

when ϱ_{xx} vanishes, so does σ_{xx} , and σ_{xy} also takes a quantized value:

$$\sigma_{xy} = -\nu \frac{e^2}{h}. \quad (24.5.5)$$

If the semiclassical expression for the off-diagonal element of the resistivity tensor were used, the equality

$$\frac{B}{n_e e} = \frac{1}{\nu} \frac{h}{e^2} \quad (24.5.6)$$

would be obtained. This would be satisfied for integer values of ν if the electron density n_e and the magnetic induction B were related by

$$n_e = \nu \frac{eB}{h}. \quad (24.5.7)$$

⁷ In two-dimensional systems the off-diagonal components of the resistance and the resistivity tensors are equal: $R_{xy} = \varrho_{xy}$. This is because $E_y = -\varrho_{xy}j_x$ leads to $V_y = -R_{xy}I_x$ via the integration of j_x and E_y in the direction perpendicular to the current flow, y .

As discussed in Section 22.1.2, the degree of degeneracy per unit surface area of the Landau levels in strong magnetic fields is given by (22.1.26), and thus

$$n_e = \nu \frac{N_p}{L_x L_y} . \quad (24.5.8)$$

Spelled out: the quantized value of the Hall resistance measured on the plateau of index ν is obtained in the semiclassical description at a particular electron density for which the lowest ν Landau levels are completely filled and all others are empty. Since elastic scattering is impossible for completely filled Landau levels, $\tau \rightarrow \infty$, and the resistivity vanishes: $\varrho_{xx} = 0$.

However, the extended character of the plateaux cannot be understood in the above picture, as the highest filled Landau level is completely filled only at very precise values of the magnetic field. Even a tiny change in the field strength modifies the degree of degeneracy of the Landau levels. With the electron number fixed, either empty states appear on the previously completely filled Landau level, or a previously empty Landau level becomes partially filled.

The resolution of this problem lies in the observation that the width of the plateaux depends strongly on the purity of the sample. In contrast to common situations, in this case the higher the impurity concentration the better. In the presence of impurities the Landau levels are broadened, as shown in Fig. 24.14. Even more important is that a part of the states are localized. These localized states do not participate in conduction: they serve as reservoirs, so the chemical potential can go continuously over from one Landau level to the other. If the field is such that the chemical potential is inside a region where the states are localized, ϱ_{xx} vanishes because these states do not contribute to the conductivity.

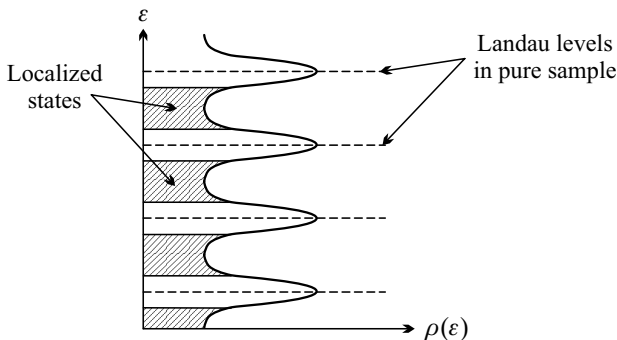


Fig. 24.14. Broadening of Landau levels and the appearance of localized states in the spectrum of a two-dimensional electron gas, due to impurities

More intriguing is the question why ϱ_{xy} takes very accurate quantized values at the same fields. To find the answer, we have to return to Chapter 22,

and continue the analysis of the electron states at the sample boundaries in strong magnetic fields. As shown in Fig. 22.7, in contrast to bulk states – whose energy depends only on the quantum number n of the Landau level and is independent of the quantum number k_y that is related to the coordinate x_0 of the oscillator centers –, the energy of the edge states (whose coordinate x_0 is close to the sample boundary) is higher. The number of branches crossing the Fermi energy is the same as the number of bulk Landau levels below the Fermi energy. Moreover, these edge states remain extended even in the presence of impurities. As their velocity is strictly directed along the edge, and they all move around the sample in the same direction, impurities cannot cause backscattering. It is as if electrons propagated in one-dimensional channels along the sample edges, without collisions.

Taking the geometry that is customarily used in the measurements of the Hall effect, the current propagates in the x -direction, and the Hall voltage is measured in the y -direction, thus the finite width of the sample is important in this direction. The gauge that is best adapted to this geometry is the Landau gauge with $\mathbf{A} = (-By, 0, 0)$. Choosing the ansatz

$$\psi(x, y) = e^{ik_x x} u(y) \quad (24.5.9)$$

for the wavefunction, the equation for $u(y)$ is

$$-\frac{\hbar^2}{2m^*} \frac{d^2 u(y)}{dy^2} + \frac{1}{2} m^* \omega_c^2 (y - y_{k_x})^2 u(y) + U(y) u(y) = \varepsilon u(y), \quad (24.5.10)$$

where $y_{k_x} = \hbar k_x / eB = k_x l_0^2$, and the potential $U(y)$ due to the finite width L_y of the sample is also taken into account. Treating this potential as a perturbation, in the first order we have

$$\varepsilon(n, k_x) = \left(n + \frac{1}{2}\right) \hbar \omega_c + U(y_{k_x}). \quad (24.5.11)$$

The electron velocities are each other's opposite for the electron states along the two edges $y_{k_x} = 0$ and $y_{k_x} = L_y$, as

$$v_x(n, k_x) = \frac{1}{\hbar} \frac{\partial \varepsilon(n, k_x)}{\partial k_x} = \frac{1}{\hbar} \frac{\partial U(y)}{\partial y} \frac{\partial y_{k_x}}{\partial k_x} = \frac{1}{eB} \frac{\partial U(y)}{\partial y}. \quad (24.5.12)$$

As we shall see in Chapter 27, electrons propagating in a one-dimensional channel contribute to the conductance by e^2/h . If there are ν Landau levels below the Fermi energy, then electrons can propagate in the same number of channels, and thus their current is

$$I_x = \nu \frac{e^2}{h} V_x. \quad (24.5.13)$$

Because of the free propagation of the electrons there is no potential drop along the sample edge. Each contact is at the same electrochemical potential

as the reservoir from which the electrons arrive. That is why ϱ_{xx} is measured to be zero in the usual setup. For the same reason, the potential difference V_y between the two sides is the same as $-V_x$, and so

$$R_{xy} = -\frac{V_y}{I_x} = \frac{1}{\nu} \frac{h}{e^2}, \quad (24.5.14)$$

in agreement with experimental findings.

It was found in measurements performed more recently on two-dimensional electron gases produced in AlGaAs/GaAs heterojunctions, which feature much higher mobilities, that the Hall resistance can take quantized values $R_{xy} = h/\nu e^2$ not only with integer values of ν but also for certain simple fractional numbers $\nu = p/q$, that is, for special fractional fillings of the highest partially filled Landau level (usually the lowest Landau level). However, the fractional quantum Hall effect (FQHE) cannot be interpreted in terms of the one-particle picture: the role of the electron–electron interaction is crucial. We shall discuss this in detail in Chapter 32.

Further Reading

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