

Exchange and Spin Interaction

The present chapter deals mainly with conduction electron scattering by centers having an uncompensated spin. Such centers are the atoms of transition and rare-earth elements (magnetic atoms); the uncompensated angular momentum of these atoms is due to the inner unfilled d- or f-shell. As to their outer valence electrons, the states of these electrons, upon saturation of chemical bonds in the crystal, are rearranged so that there are two electrons of opposite spin in each state.

Magnetic atoms can be the host atoms of the lattice of an ideal crystal or can be impurities in a lattice of nonmagnetic atoms.

Relevant in many cases in the present chapter is that not only the scattering center, but the band electron has a spin as well. Consequently, the data in this chapter are closely related to those of ch. 13.

15.1. Interaction between a conduction electron and a magnetic atom

We begin by considering the Coulomb interaction energy of two electrons: a band electron in state $\psi(\mathbf{r})$ with the spin projection σ , and one of the electrons in a magnetic atom, with the electron in the state $\varphi(\mathbf{r})$ with the spin projection μ . This energy is

$$\begin{aligned} & \langle \psi\sigma, \varphi\mu | e^2/r_{12} | \psi\sigma, \varphi\mu \rangle - \langle \psi\sigma, \varphi\mu | e^2/r_{12} | \varphi\mu, \psi\sigma \rangle \\ &= \int d^3r \int d^3r' \psi^*(\mathbf{r}) \varphi^*(\mathbf{r}') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \psi(\mathbf{r}) \varphi(\mathbf{r}') \\ & \quad - \delta_{\sigma,\mu} \int d^3r \int d^3r' \psi^*(\mathbf{r}) \varphi^*(\mathbf{r}') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \varphi(\mathbf{r}) \psi(\mathbf{r}'). \end{aligned} \quad (15.1)$$

The first term is the so-called direct interaction, the second term is the exchange interaction. The direct interaction is independent of the spin orientations; the exchange interaction exists only for electrons with the same spin orientations (the Pauli exclusion principle “does not work” for electrons with different spin orientations).

We can write the energy given by eq. (15.1) in the form

$$\int d^3r \psi^*(\mathbf{r}) \hat{v}_\varphi \psi(\mathbf{r}). \quad (15.2)$$

Here \hat{v}_φ is the effective field set up by the atomic electron for the band electron. It is evident from eq. (15.1) that

$$\hat{v}_\varphi = V_\varphi(\mathbf{r}) - \delta_{\sigma,\mu} \hat{A}_\varphi. \quad (15.3)$$

Here V_φ is the potential set up by the electron in the state φ , i.e.

$$V_\varphi(\mathbf{r}) = \int d^3r' \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} |\varphi(\mathbf{r}')|^2; \quad (15.4)$$

this potential is responsible for the direct Coulomb interaction. Responsible for the exchange interaction is the integral operator \hat{A}_φ , which acts as follows:

$$\hat{A}_\varphi \psi(\mathbf{r}) \equiv \int d^3r' \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \varphi^*(\mathbf{r}') \varphi(\mathbf{r}) \psi(\mathbf{r}'), \quad (15.5)$$

i.e. \hat{A}_φ is an integral operator with kernel

$$A_\varphi(\mathbf{r}, \mathbf{r}') = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \varphi^*(\mathbf{r}') \varphi(\mathbf{r}). \quad (15.6)$$

It sometimes proves convenient, for the sake of generality, to understand the potential V_φ as also being an integral operator, but with a diagonal kernel

$$V_\varphi(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') V_\varphi(\mathbf{r}). \quad (15.7)$$

The Kronecker delta appearing in eq. (15.3) can be represented as an "interaction of spins", by writing

$$\hat{v}_\varphi = V_\varphi(\mathbf{r}) - \frac{1}{2}(1 + 4\mathbf{s}'\mathbf{s}) \hat{A}_\varphi, \quad (15.8)$$

where \mathbf{s} and \mathbf{s}' are operators of the band and atomic electron spins. The potential given by eq. (15.8) is the operator acting on the spinor-column of the band electron.

After summing the interactions \hat{v}_φ eq. (15.8) for all the electrons of the magnetic atom, and also taking into account the interaction of the band electron with the atomic nucleus, we write the Hamiltonian for the interaction of the band electron with a magnetic atom in the form

$$\hat{\mathcal{H}} = \hat{Q} + \hat{\mathbf{R}}\mathbf{s}. \quad (15.9)$$

Two parts of this interaction are distinguished: the part depending and the part not depending on the spin of the band electron. The operators \hat{Q} and $\hat{\mathbf{R}}$ are, in general, integral operators, with kernels $Q(\mathbf{r}, \mathbf{r}')$ and $\mathbf{R}(\mathbf{r}, \mathbf{r}')$, which include both diagonal and nondiagonal parts. For example,

$$Q(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') Q_1(\mathbf{r}) + Q_2(\mathbf{r}-\mathbf{r}'). \quad (15.10)$$

The diagonal part $Q_1(\mathbf{r})$ includes the potential of the electron cloud of the magnetic atom and of its nucleus. Hence, $Q_1(\mathbf{r})$ is a potential set up by an electrically neutral formation and is therefore a short-range one. The diagonal part \mathbf{R}_1 represents the spin-orbit interaction of the band electron in the field of the nucleus and in the field of the electron cloud [see eq. (13.8)].

The nondiagonal parts Q_2 and \mathbf{R}_2 are responsible for the exchange interaction. The exchange interaction Q_2 , which is independent of spin orientation, can be understood as being the interaction with the atomic states occupied by two electrons with opposite spins. The exchange interaction with spin-nonsaturated states is included in \mathbf{R}_2 . The spin-orbit interaction in the "exchange field" of the atom can also be included in \mathbf{R}_2 , but it is usually neglected.

Hamiltonian (15.9) is substantially simplified if the conduction electron wavelength $2\pi/k$ is much longer than the dimension a^* of the magnetic atom. Then the matrix element of the operator \hat{Q} , calculated with the two functions, $\psi'(\mathbf{r})$ and $\psi(\mathbf{r})$, can be represented as follows:

$$\int d^3r \psi'(\mathbf{r}) \hat{Q} \psi(\mathbf{r}) \approx Q \psi'(0) \psi(0), \quad (15.11)$$

where the point $\mathbf{r} = 0$ is the center of the atom and Q is the number:

$$\begin{aligned} Q &= \int d^3r \int d^3r' Q(\mathbf{r}, \mathbf{r}') \\ &= \int d^3r Q_1(\mathbf{r}) + \int d^3r \int d^3r' Q_2(\mathbf{r}, \mathbf{r}'). \end{aligned} \quad (15.12)$$

An approximation of the type of eq. (15.11) for the matrix elements of the operators \hat{Q} and $\hat{\mathbf{R}}$ corresponds to the Hamiltonian

$$\mathcal{H} = (Q + \mathbf{R} \cdot \mathbf{s}) \delta(\mathbf{r}), \quad (15.13)$$

in which Q and \mathbf{R} are no longer operators; they are a number and a vector, respectively.

The vector \mathbf{R} , as follows from the aforesaid, is related to the state of the inner unfilled d- or f-shell. In a free atom the state of this shell is characterized by the orbital angular momentum \mathbf{L} , spin angular momentum \mathbf{S} and the total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$. The d-shell electrons of a magnetic atom in a crystal are usually in a strong crystalline field due to the surrounding atoms. This field impedes free rotation of the angular momentum \mathbf{L} , so that it is "frozen", in effect, to the value $\mathbf{L} = 0$. In this case the vector \mathbf{R} is directed along \mathbf{S} , so that the spin part of Hamiltonian (15.13) is of the form $A \mathbf{S} \cdot \mathbf{s} \delta(\mathbf{r})$, where A is a certain constant that characterizes the exchange interaction of the band electron with one unpaired electron of the inner shell. Such an interaction is said to be the exchange interaction of a conduction-electron spin with the spin of localized electrons. The crystalline field is of no importance for the f-shell electrons and, strictly speaking, $\mathbf{L} \neq 0$. It is natural to replace in this

case the vector \mathbf{S} in the exchange Hamiltonian by its projection onto \mathbf{J} , i.e. by $(g-1)\mathbf{J}$, where g is the g -factor of the f -shell. As a matter of fact, when $L=0$ (the magnetic moment of the f -shell is purely of the spin type), $g=2$, and $(g-1)\mathbf{J}$ is simply equal to \mathbf{S} . When $\mathbf{S}=0$ (the magnetic moment of the shell is purely of the orbital type), $g=1$, and the exchange interaction, which depends upon spin, vanishes, as it should.

Sometimes, to take the finite dimensions of the magnetic atom into account, the interaction is assumed in the form

$$\mathcal{J}(\mathbf{r}) \mathbf{S} \mathbf{s}, \quad (15.14)$$

where $\mathcal{J}(\mathbf{r})$ is the so-called exchange integral. Note, however, that the representation given by eq. (15.14) is a model representation and cannot be obtained from eq. (15.9) by any step-by-step procedure whatsoever.

The magnitude of the exchange integral is of the order of the atomic energy of the inner shell with radius a^* , i.e.

$$\mathcal{J} \sim \varepsilon_0, \quad A \sim \varepsilon_0 (a^*)^3, \quad (15.15)$$

where ε_0 is an energy of the order of e^2/a^* .

The amplitude of the scattering $\mathbf{k} \rightarrow \mathbf{k}'$, corresponding to perturbation (15.9), can be written in the form

$$f_{\mathbf{k}' \rightarrow \mathbf{k}} = A_{\mathbf{k}'\mathbf{k}} + \mathbf{B}_{\mathbf{k}'\mathbf{k}} \mathbf{S}. \quad (15.16)$$

In the Born approximation

$$A_{\mathbf{k}'\mathbf{k}} = -\frac{m}{2\pi\hbar^2} \int d^3r e^{-i\mathbf{k}'\mathbf{r}} \hat{Q} e^{i\mathbf{k}\mathbf{r}}, \quad (15.17)$$

$$\mathbf{B}_{\mathbf{k}'\mathbf{k}} = -\frac{m}{2\pi\hbar^2} \int d^3r e^{-i\mathbf{k}'\mathbf{r}} \hat{\mathbf{R}} e^{i\mathbf{k}\mathbf{r}}. \quad (15.18)$$

The simplification of Hamiltonian (15.9), associated with the large conduction-electron wavelength, in terms of the scattering amplitude f , involves its expansion for small \mathbf{k} and \mathbf{k}' . A Hamiltonian in the form of eq. (15.13) corresponds to the fact that $A_{\mathbf{k}'\mathbf{k}}$ and $\mathbf{B}_{\mathbf{k}'\mathbf{k}}$ are considered to be independent of \mathbf{k} and \mathbf{k}' . The exchange interaction, when written in the form of eq. (15.14), corresponds to $\mathbf{B}_{\mathbf{k}'\mathbf{k}}$, which depends only on $\mathbf{q} = \mathbf{k}' - \mathbf{k}$.

15.2. Scattering by a spin lattice

When the magnetic atoms are the host atoms and are arranged in space in an ordered fashion, the only random element leading to scattering is the random orientation of the spins of the various atoms. Therefore, conduction electron scattering is determined by the spin part of perturbation (15.9):

$$\mathcal{H} = \sum_{\mathbf{a}} \mathcal{J}(\mathbf{r} - \mathbf{a}) \mathbf{S}_{\mathbf{a}} \mathbf{s}. \quad (15.19)$$

Here \mathbf{a} is a vector of the lattice at whose sites the magnetic atoms (taken, for simplicity, to be identical) are located. For the sake of clarity, the spins \mathbf{S}_a are assumed to be classical quantities. Owing to the interaction with a thermal bath, for example with phonons, each spin \mathbf{S}_a fluctuates with time and is a random stationary function $\mathbf{S}_a(t)$ of time. If the spin lattice is disordered (paramagnetic), the average over time is $\langle \mathbf{S}_a \rangle = 0$. But if the lattice is ordered, then $\langle \mathbf{S}_a \rangle \neq 0$; in ferromagnetic ordering this average $\langle \mathbf{S}_a \rangle = \langle \mathbf{S} \rangle$ is the same for all lattice sites \mathbf{a} .

For a ferromagnetically ordered lattice, perturbation (15.19) includes the nonfluctuating component

$$\langle \mathcal{H} \rangle = \sum_a \mathcal{J}(\mathbf{r} - \mathbf{a}) \langle \mathbf{S} \rangle s, \quad (15.20)$$

which is periodic in space. This component should be included in the Hamiltonian that determines the band structure. It leads to band splitting with respect to the conduction-electron spin orientation relative to $\langle \mathbf{S} \rangle$. The cause of the scattering is only the fluctuating part of perturbation (15.19) (Kasuya 1956, de Gennes and Friedel 1958), namely

$$\delta \mathcal{H} = \sum_a \mathcal{J}(\mathbf{r} - \mathbf{a}) \delta \mathbf{S}_a s, \quad (15.21)$$

where the spin fluctuation of a magnetic atom is

$$\delta \mathbf{S}_a = \mathbf{S}_a - \langle \mathbf{S} \rangle. \quad (15.22)$$

15.2.1. Scattering probability

Let us calculate the probability of the scattering $\sigma \mathbf{k} \rightarrow \sigma' \mathbf{k}'$, due to the perturbation given by eq. (15.21). As the wave functions of the band electron we take (neglecting the spin-orbit interaction in band formation, see sect. 1.1)

$$\frac{1}{L^{3/2}} u_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}} |\sigma\rangle, \quad (15.23)$$

where $u_{\mathbf{k}}$ is the Bloch factor and $|\sigma\rangle$ is a spinor corresponding to the orientation σ of the electron spin. If the spin lattice is paramagnetic, states (15.23) with different σ pertain to the same energy $\epsilon_{\mathbf{k}}$ and the quantization axis of the conduction-electron spin is arbitrary. For a ferromagnetic lattice, the quantization axis z is determined by the direction of the "average magnetization" $\langle \mathbf{S} \rangle$, and states with different spin orientations are split by perturbation (15.20), i.e.

$$\epsilon_{\sigma \mathbf{k}} = \epsilon_{\mathbf{k}} \pm N \mathcal{J}_{\mathbf{k}, \mathbf{k}} \langle S_z \rangle. \quad (15.24)$$

Here $\epsilon_{\mathbf{k}}$ is the electron band without taking perturbation (15.20) into account,

and N is the number of magnetic atoms per unit volume (with one magnetic atom per unit cell, $N = a_0^{-3}$),

$$\mathcal{J}_{k,k} = \int_{\infty} d^3r |u_k(\mathbf{r})|^2 \mathcal{J}(\mathbf{r}), \tag{15.25}$$

with the plus sign in eq. (15.24) referring to the spin orientation $\sigma = \uparrow$ and the minus referring to the orientation $\sigma = \downarrow$.

The scattering matrix element calculated with functions (15.23) can be brought, making use of the periodicity of the Bloch factors, to the form

$$M_{\sigma'k',\sigma k} = \frac{1}{L^3} \mathcal{J}_{k,k'} \langle \sigma' | s | \sigma \rangle \sum_a e^{-iqa} \delta S_a, \tag{15.26}$$

where

$$\begin{aligned} \mathcal{J}_{k,k'} &= \int_{\infty} d^3r e^{-iqr} u_{k'}^*(\mathbf{r}) u_k(\mathbf{r}) \mathcal{J}(\mathbf{r}) \\ &= \mathcal{J}_{k',k}^*, \end{aligned} \tag{15.27}$$

where $\mathbf{q} = \mathbf{k}' - \mathbf{k}$. In order to calculate the scattering probability by means of eq. (2.109), we determine the correlator of such matrix elements:

$$\begin{aligned} \langle M_{\sigma'k',\sigma k}^*(0) M_{\sigma'k',\sigma k}(t) \rangle &= \frac{1}{L^6} |\mathcal{J}_{k,k'}|^2 \langle \sigma' | s_i | \sigma \rangle^* \langle \sigma' | s_j | \sigma \rangle \\ &\quad \times \sum_{aa'} e^{i\mathbf{q}(a-a')} \langle \delta S_a^i(0) \delta S_{a'}^j(t) \rangle. \end{aligned} \tag{15.28}$$

Here i and j are the Cartesian indices x , y and z . Included in the expression obtained above is the time correlator of the spins at the various lattice sites. By virtue of translational symmetry, the correlator depends only on the difference $a - a'$. Making use of eq. (2.110) we have

$$\begin{aligned} W_{\sigma k \rightarrow \sigma' k'} &= \frac{1}{L^3} N \frac{1}{\hbar^2} |\mathcal{J}_{k,k'}|^2 \langle \sigma' | s_i | \sigma \rangle^* \langle \sigma' | s_j | \sigma \rangle \langle \delta S^i \delta S^j \rangle_{q\omega}, \\ \mathbf{q} = \mathbf{k}' - \mathbf{k}, \quad \hbar\omega &= \varepsilon_{\sigma'k'} - \varepsilon_{\sigma k}, \end{aligned} \tag{15.29}$$

where

$$\langle \delta S^i \delta S^j \rangle_{q\omega} = \int_{-\infty}^{\infty} dt e^{i\omega t} \sum_a e^{-iqa} \langle \delta S_0^i(0) \delta S_a^j(t) \rangle. \tag{15.30}$$

After introducing the explicit matrix elements of the conduction-electron spin, the final results obtained are (Haas 1968):

$$W_{\uparrow k \rightarrow \uparrow k'} = W_{\downarrow k \rightarrow \downarrow k'} = B_{k,k'} \langle \delta S \delta S \rangle_{q\omega}^{\parallel} \tag{15.31}$$

for the probability of scattering without spin-flip, and

$$W_{\uparrow k \rightarrow \downarrow k'} = W_{\downarrow k \rightarrow \uparrow k'} = B_{k,k'} \langle \delta S \delta S \rangle_{q\omega}^{\perp} \quad (15.32)$$

for the probability of scattering with spin-flip. For the sake of brevity, we have used the notation

$$B_{k,k'} = \frac{1}{L^3} N \frac{1}{4\hbar^2} |\mathcal{J}_{k,k'}|^2 \quad (15.33)$$

and have introduced the Fourier components of the correlators for the longitudinal and transverse components of the atomic spin (with respect to the quantization axis of the band electron spin):

$$\langle \delta S \delta S \rangle^{\parallel} = \langle \delta S^z \delta S^z \rangle, \quad (15.34)$$

$$\langle \delta S \delta S \rangle^{\perp} = \langle \delta S^- \delta S^+ \rangle = \langle \delta S^+ \delta S^- \rangle, \quad (15.35)$$

where $\delta S^{\pm} = \delta S^x \pm i\delta S^y$, and the indices $q\omega$ have been omitted for the sake of brevity.

For the case when band splitting with respect to spin is absent or can be neglected, it proves beneficial to deal with a scattering probability that has been averaged over the initial orientations σ and summed over the final orientations σ' . Thus

$$\begin{aligned} W_{k \rightarrow k'} &= \frac{1}{2} \sum_{\sigma\sigma'} W_{\sigma k \rightarrow \sigma' k'} \\ &= B_{k,k'} \langle (\delta S)^2 \rangle_{q\omega}. \end{aligned} \quad (15.36)$$

If it is necessary to take into account quantum effects that are associated with the noncommutativity of the various atomic spin components, the averages appearing in the definition of the transverse correlator in eq. (15.35) are no longer equal. Then, instead of eq. (15.32), we have

$$\begin{aligned} W_{\uparrow k \rightarrow \downarrow k'} &= B_{k,k'} \langle \delta S^- \delta S^+ \rangle_{q\omega}, \\ W_{\downarrow k \rightarrow \uparrow k'} &= B_{k,k'} \langle \delta S^+ \delta S^- \rangle_{q\omega}, \end{aligned} \quad (15.37)$$

i.e. the probability of a spin-flip transition depends upon the initial projection of the band electron spin along the direction of $\langle \mathbf{S} \rangle$.

Equations (15.31) and (15.37) are highly general and describe electron scattering in the Born approximation by a spin lattice in an arbitrary state. This state is formed both by the interaction of the spins with one another and by their interaction with a thermal bath (phonons). The equations are also valid in the case when the system is placed in an external magnetic field \mathbf{H} (provided this field does not lead to quantization of orbital motion of the band electron; see sect. 14.1). But the calculation of spin correlators is an extremely complex problem of magnetism theory; its complete solution is as yet unknown. Therefore, the following discussion concerns various states of the spin

lattice for which it is possible to find some approximate equations for the spin correlators.

Recall that the Fourier component of the spin correlator given by eq. (15.30) is related to the magnetic susceptibility χ of the spin lattice, with the susceptibility being the reaction to an external magnetic field with frequency ω and period $2\pi/q$. This susceptibility is

$$\chi_{q\omega}^{ij} = \frac{(g\mu_B)^2}{T} \langle \delta S^i \delta S^j \rangle_{q\omega}. \quad (15.38)$$

This equation includes the Bohr magneton μ_B and the g -factor of the atomic spin. The susceptibility χ is given per magnetic atom. Sometimes relation (15.38) enables experimental data on conductivity to be tied in with the results of susceptibility measurements.

15.2.2. The paramagnetic region – $T > T_c$

In the paramagnetic region (at sufficiently high temperatures) the spins at the various lattice sites can be assumed to be noninteracting, for which reason they do not correlate, i.e.

$$\langle \delta S_a^i(0) \delta S_{a'}^j(t) \rangle = \delta_{aa'} \langle \delta S^i(0) \delta S^j(t) \rangle, \quad (15.39)$$

in which the index a is omitted in the correlator because the correlator is the same for all the sites. Then, from eq. (15.30), we have

$$\begin{aligned} \langle \delta S^i \delta S^j \rangle_{q\omega} &= \langle \delta S^i \delta S^j \rangle_{\omega} \\ &\equiv \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \delta S^i(0) \delta S^j(t) \rangle. \end{aligned} \quad (15.40)$$

The dependence of a one-site correlator as given by eq. (15.39) on time is determined by the forces that make the spin rotate: the external magnetic field H and the interaction with lattice vibrations. If only the field H is taken into account, one-site correlators are readily calculated:

$$\begin{aligned} \langle \delta S^z \delta S^z \rangle_{\omega} &= 2\pi \delta(\omega) \langle (\delta S^z)^2 \rangle, \\ \langle \delta S^- \delta S^+ \rangle_{\omega} &= 2\pi \delta(\omega - \omega_Z) \langle \delta S^- \delta S^+ \rangle, \\ \langle \delta S^+ \delta S^- \rangle_{\omega} &= 2\pi \delta(\omega + \omega_Z) \langle \delta S^+ \delta S^- \rangle, \end{aligned} \quad (15.41)$$

Here $\hbar\omega_Z = g\mu_B H$ is the Zeeman splitting of the atomic spin in the field H , and the angular brackets with no indices denote one-site single-time corre-

lators (both quantities being taken at $t = 0$), known from elementary magnetism theory:

$$\begin{aligned} \langle (\delta S^z)^2 \rangle &= S(S+1) + \langle S^z \rangle \coth \frac{1}{2}\beta - \langle S^z \rangle^2, \\ \langle \delta S^\mp \delta S^\pm \rangle &= -\langle S^z \rangle (\coth \frac{1}{2}\beta \mp 1), \\ \langle S^z \rangle &= -SB_S(\beta), \quad \langle S^\pm \rangle = \langle S^\mp \rangle = 0. \end{aligned} \quad (15.42)$$

Here B_S is the Brillouin function

$$B_S(\beta) = \frac{2S+1}{2S} \coth \left(\frac{2S+1}{2S} \beta \right) - \frac{1}{2S} \coth \left(\frac{1}{2S} \beta \right), \quad (15.43)$$

where $\beta = g\mu_B H/T$.

Electron scattering without spin-flip is elastic because the projection S^z of the atomic spin and its Zeeman energy are conserved. Spin-flip scattering is accompanied by an energy transfer equal to the Zeeman splitting $g\mu_B H$.

At $H=0$ all electron scattering events are elastic, and the averaged probability, eq. (15.36), as is readily evident from eqs. (15.40) and (15.41), is

$$W_{k \rightarrow k'} = 2\pi \delta(\omega) B_{k,k'} S(S+1). \quad (15.44)$$

This probability is independent of temperature.

When the radius a^* of the inner shell of the magnetic atom is much smaller than the characteristic wavelength $2\pi/k$ of the band electron, we can replace $\mathcal{J}(\mathbf{r})$ by $A\delta(\mathbf{r})$ in calculating $\mathcal{J}_{k,k'}$. Then

$$|\mathcal{J}_{k,k'}|^2 = |A|^2 |u_k(0)|^2 |u_{k'}(0)|^2, \quad (15.45)$$

where the point $\mathbf{r} = 0$ corresponds to the position of the magnetic atom. In this approximation, scattering probability (15.44) is of a separable form on the constant-energy surface, i.e. it takes the form

$$W_{k \rightarrow k'} = \delta(\varepsilon_k - \varepsilon_{k'}) a_k a_{k'}. \quad (15.46)$$

The coefficients a_k are even function of \mathbf{k} , i.e. $a_k = a_{-k}$. This stems from the properties of the Bloch functions

$$u_{-\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}^*(\mathbf{r}), \quad (15.47)$$

which follows from eq. (1.6). After making use, in addition, of eq. (1.7), it is evident that in the approximation of a small radius of the magnetic atom, spin scattering is randomizing in the sense of eq. (2.98). Valid for spin scattering in calculating the current in a weak electric field is the τ -approximation with the scattering time

$$\begin{aligned} \frac{1}{\tau(\mathbf{k})} &= \sum_{k'} W_{k \rightarrow k'} \\ &= \frac{1}{2} \pi N \hbar^3 S(S+1) |A|^2 |u_k(0)|^2 \overline{|u(0)|^2}^{\varepsilon} g(\varepsilon). \end{aligned} \quad (15.48)$$

Here $g(\epsilon)$ is the density of states, and the overbar denotes averaging over the constant-energy surface in accordance with eq. (2.68).

The average $\overline{|u|^2}^\epsilon$ for a metal can be taken at $\epsilon = \epsilon_F$, including this constant factor in the constant $|A|^2$. In a semiconductor, in which \mathbf{k} and $\epsilon_{\mathbf{k}}$ are always in a small region of the BZ close to \mathbf{k}_0 , we can calculate $\overline{|u_{\mathbf{k}}|^2}$ at $\mathbf{k} = \mathbf{k}_0$ (if \mathbf{k}_0 is not a point of degeneracy, see sect. 1.1), and the average $\overline{|u|^2}^\epsilon$ at $\epsilon = \epsilon_0$, where \mathbf{k}_0 and ϵ_0 correspond to the bottom (or top) of the band. The two Bloch factors are equal in this case and can be included in $|A|^2$; the scattering is found to be isotropic.

15.2.3. The ferromagnetic region – $T < T_c$

In the ferromagnetic region, far from the transition point T_c , the fluctuations of the atomic spins are small, and electron scattering by spin disorder is weak. This scattering can be described as emission and absorption of magnons (see, e.g., Korenblit and Lazarenko 1971). In scattering by magnons, the correlators appearing in probability (15.37) of spin-flip scattering are the following:

$$\begin{aligned}\langle \delta S^- \delta S^+ \rangle_{q\omega} &= 2S\delta(\omega - \omega_q) N_q, \\ \langle \delta S^+ \delta S^- \rangle_{q\omega} &= 2S\delta(\omega + \omega_q) (N_q + 1).\end{aligned}\tag{15.49}$$

Here $\hbar\omega_q$ is the energy of a magnon having the wavevector \mathbf{q} , and N_q are the equilibrium magnon occupation numbers, which are given by the same Planck function, eq. (3.11), as for phonons. After substituting eq. (15.49) into eq. (15.37), we obtain an expression for the transition probability that is of the same structure as eq. (3.8) for phonon scattering. Since the magnon has an angular momentum projection onto the direction of $\langle \mathbf{S} \rangle$ equal to -1 , it is clear that the scattering of a band electron by magnons without spin-flip is impossible.

All that was stated in sect. 3.1 in connection with the electron–phonon interaction, about spontaneous and induced scattering, is valid for magnon scattering. In particular, spontaneous emission of magnons by a hot electron is possible at a spin lattice temperature $T=0$. This process can be treated as electron scattering by zero-point vibrations of the system of atomic spins.

Considered above was the simplest situation: one spin in a primitive cell and ferromagnetic ordering. In the case of cells containing several spins, a contribution to scattering is made by correlators of the types given by eq. (15.34) and (15.35) for spins of various kinds, as well as by crossed correlators. Correspondingly, several magnon branches appear. Scattering probability calculations become more cumbersome, but they can be carried out by the same methods.

Frequently applied, for the sake of simplicity, is an isotropic model of scattering by magnons, devised by analogy with the isotropic model of

scattering by phonons described in ch. 4. Two types of magnon dispersion laws are considered:

$$\hbar\omega_q = \Delta + \hbar^2 q^2 / 2m^*, \quad (15.50)$$

$$\hbar\omega_q = \Delta + \hbar s^* q. \quad (15.51)$$

The quadratic dispersion law is typical for ferromagnetic materials, the linear law, for antiferromagnetic materials. The gap $\Delta \neq 0$ if there is intrinsic anisotropy or anisotropy due to an external magnetic field. From experimental data it is known that in the majority of cases the energy scale of magnons is the same as for phonons. The description of scattering as emission and absorption of magnons is of advantage only at low temperatures. It is clear, by analogy with phonons, that only long-wavelength magnons with $q \ll b_0$ are of importance under these conditions. Matrix elements for the emission and absorption of long-wavelength magnons (averaged over the electron spin orientations) can be written in the form of eq. (4.1). Here the dependence of $B(q)$ on q differs for magnons of various types:

$$B(q) = B_0 \quad \text{for ferromagnons,} \quad (15.52)$$

$$B(q) = B_0 q \quad \text{for antiferromagnons.} \quad (15.53)$$

Approximation (15.52) is confirmed by eq. (15.33): as $q \rightarrow 0$, the factor $B_{k,k'}$ remains finite. In antiferromagnetic substances, the scattering matrix element vanishes as $q \rightarrow 0$ because the perturbations produced by two opposite spins in a primitive cell are mutually cancelled.

15.2.4. The critical region – $T \approx T_c$

It proves most complex to describe scattering near the transition point T_c . If we approach T_c from the paramagnetic region, the interaction between separate atomic spins becomes of importance, whereas if we approach T_c from the ferromagnetic region, the interaction between spin waves becomes relevant.

A discussion of the degree of reliability of various approximations for the spin correlator near the transition point is outside the scope of the present book. But all theoretical considerations indicate that as $T \rightarrow T_c$, spin fluctuations increase drastically; this concerns long-wavelength and low-frequency fluctuations with $q \ll \pi/d$ and $\omega \ll \mathcal{J}/\hbar$. Here d is the average distance between spins and \mathcal{J} is the energy of their interaction (of the order of T_c). If small momentum and energy transfers are of importance in electron scattering, then scattering in the vicinity of the critical point greatly increases. But if small transfers turn out to disagree with the conservation laws (see sect. 2.6), no increase in scattering occurs near T_c . This is illustrated by fig. 15.1, which shows the dependence of the scattering rate on the temperature for an electron with wavevector k for various values of kd , where d is the spin lattice

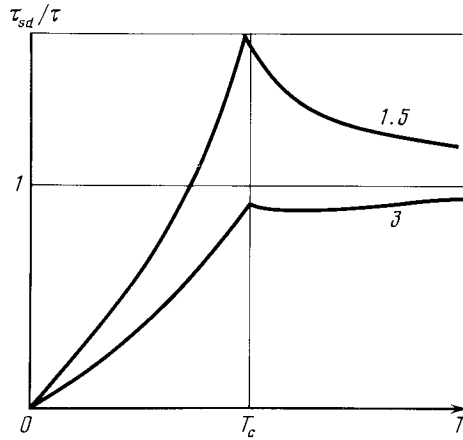


Fig. 15.1. Temperature dependence of the rate of elastic scattering by a spin lattice; τ_{sd} is the spin-disorder scattering time, τ is determined by eq. (15.48); kd values are shown near the curves (de Gennes and Friedel 1958).

constant. The scattering is assumed to be elastic, and the correlation function is calculated according to molecular field theory.

The resistivity in a Fermi gas is determined by τ at $k = k_F$. It is evident, therefore, from fig. 15.1 that only in the case when the magnetic atoms are sufficiently densely arranged, $k_F d \leq \pi$, does the increase in fluctuations in the vicinity of T_c manifest itself as a maximum in the resistivity. The wavevector k is small in semiconductors and therefore a maximum in the resistivity is usually exhibited [see, for example, the relation $\rho(T)$ for EuO (Shapira et al. 1973)].

15.2.5. Electrical resistivity of rare-earth metals

A brief review of experimental data on the electrical resistivity of rare-earth metals is given below to illustrate the theoretical formulas of the preceding subsection. The temperature dependences of the electrical resistivity of a group of heavy rare-earth metals, from gadolinium through thulium, are given in fig. 15.2. All of these elements have hexagonal close-packed lattices with values of the lattice constants very close to each other, an equal number of valence electrons and, consequently, with very similar FS. The main difference between these elements is the filling of the 4f-shell. Consequently, they have different magnetic ordering temperatures T_c , which are shown, in the figure, near the curves. The ordered structures themselves also differ from one another. Directly below T_c , in most of these elements various types of periodic magnetic structures occur. Their spacing is, in general, incommensurate with the lattice constant and depends upon temperature. As a result, not only

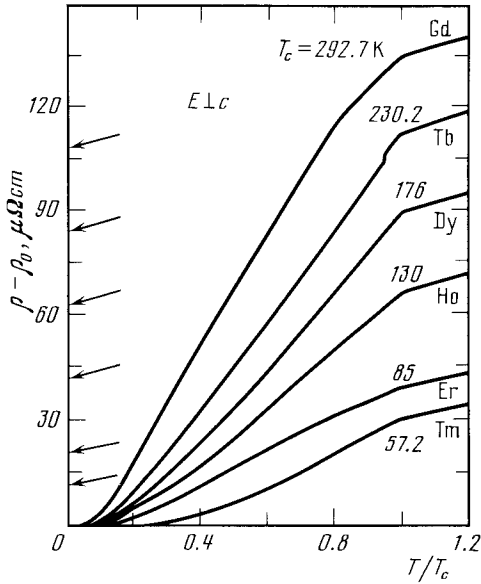


Fig. 15.2. Temperature dependences of the electrical resistivity of rare-earth metals (Legvold 1972).

scattering varies with temperature, but also the electron band structure itself. This considerably complicates the interpretation of experimental data. Hence we shall not discuss the region $T \sim T_c$ here. At $T \ll T_c$ the magnetic structures are stabilized.

Let us begin with the paramagnetic region $T > T_c$ (Legvold 1972). In the relaxation-time approximation, the electrical resistivity is the sum of three resistivities: the residual resistivity ρ_0 , the spin-disorder resistivity ρ_{sd} , which, according to eq. (15.48), is independent of T , and the phonon resistivity ρ_{ph} , which varies linearly with temperature [see eq. (4.66); we can put $\rho_{ph} \propto T$ because the lowest magnetic transition temperature, that of thulium, is, nevertheless, not very low: about 60 K, i.e. comparable to the Debye temperature T_D]. After measuring ρ_0 and extrapolating the linear, high-temperature dependence $\rho - \rho_0$ on T to zero temperature, we obtain the value of ρ_{sd} . This quantity is indicated on the ordinate axis by arrows for all seven metals. Similar measurements were also carried out with the electric field in the direction $\mathbf{E} \parallel c$.

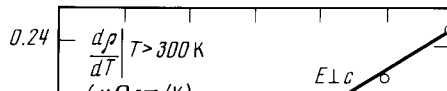
By making use of eq. (7.4), the measured values of ρ_{sd} can be converted to $1/\tau$. The latter should be compared to the result obtained by eq. (15.48), in which, however, the factor $S(S+1)$ should be replaced by $(g-1)^2 J(J+1)$, in accordance with what was said in sect. 15.1 about the meaning of the vector \mathbf{R} in eq. (15.13).

Summarizing, the expression for ρ_{sd} includes, in addition to the factor $(g-1)^2 J(J+1)$, whose presence is precisely what is subject to experimental verification, the integral

$$I_E = \int_{FS} v_E dS_E$$

from eq. (7.4) (the index E denotes the projection on the direction of the electric field), as well as several factors from eq. (15.48). Since the band structure of all the metals being discussed is practically the same, it follows that the variation of both the quantity A and the Bloch factors in going from one metal to another should be small. This, as we shall see in the following, is experimentally confirmed. The changes in the quantity I_E can be taken into account as follows. A measurement of the FS indicates that its changes from one element to another consist mainly in the change in the diameter of its "trunk", which is oriented along the c axis and provides for openness of the FS in this direction. Such a change in the FS should mainly affect the integral I_E when $E \perp c$. This consideration can be directly compared with experimental data because the parameter I_E appears, not only in the spin disorder resistivity, but in the phonon resistivity as well. The latter is characterized by the coefficient of the linear term in ρ in the temperature region $T > T_c$. As is evident from the curves in fig. 15.3, the quantity $d\rho/dT$ really does vary comparatively little when $E \parallel c$ along the series from Gd through Tm.

The quantity ρ_{ph} depends not only on I_E but on other factors as well, for instance, the changes in the phonon spectrum. In the simplest case, for the isotropic model, the phonon spectrum enters into the expression for $1/\tau$ through the sound velocity s [see eq. (4.66)], but in the anisotropic model, its influence is not so simply taken into consideration. Legvold (1972) assumed



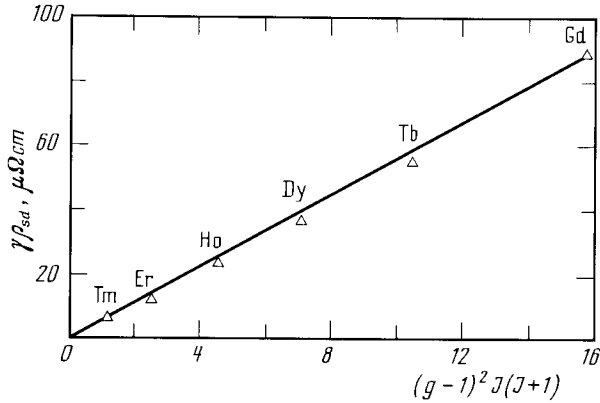


Fig. 15.4. Paramagnetic resistivity of rare-earth metals multiplied by a factor taking into account the area of the FS as a function of the quantity $(g-1)^2 J(J+1)$ (Legvold 1972).

that the slight variation in $d\rho/dT$ along the series from Gd through Tm for $\mathbf{E} \parallel c$ occurs only due to the changes in the phonon spectrum. Then the much larger variations of $d\rho/dT$ in the basal plane should be attributed to changes in the parameter I_E , and should be taken into account in the analysis of ρ_{sd} . Hence, the values of ρ_{sd} , taken from fig. 15.2, are multiplied in fig. 15.4 by the ratio $(d\rho/dT)_{\parallel} / (d\rho/dT)_{\perp}$. As is evident from the curve, the quantity ρ_{sd} , corrected in this way, turns out to be proportional to $(g-1)^2 J(J+1)$, which was to be proved. This indirectly confirmed the previously proposed natural assumption that all the other factors in eq. (15.48) do not vary along the series of elements from Gd through Tm.

The possibilities of experimental investigations in the scattering of electrons by magnons are usually drastically restricted due to the masking effect of phonon scattering. This may be illustrated by measurements of the electrical resistivity of Tb below 50 K made by Andersen and Smith (1979). In this region, Tb has an anisotropic ferromagnetic structure, enabling eq. (15.52) to be employed as the interaction matrix element. The magnon spectrum has the form of eq. (15.50), where the quantities Δ and m^* are known from neutron measurements ($\Delta \approx 19$ K). After substituting $B(q)$ and $\omega(q)$ into eq. (4.59), we can calculate the temperature dependence of magnon scattering:

$$\frac{1}{\tau_1^{\text{mag}}} \propto \begin{cases} T \exp(-\Delta/T), & \text{for } T \ll \Delta, \\ T^2, & \text{for } T \gg \Delta. \end{cases} \quad (15.54)$$

But the proportionality factor is inadequately known. Even if the value of ρ_{sd} measured for Tb is used (see fig. 15.5) to eliminate in ρ_{mag} the uncertainty associated with the intensity of the magnetic interaction, there still remains a factor, determined by the electron band structure and difficult to calculate (in

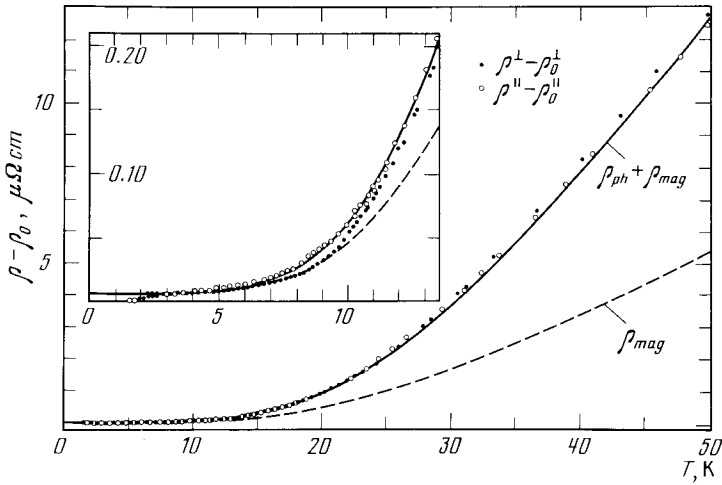


Fig. 15.5. Calculated and measured temperature dependence of the electrical resistivity of Tb. The solid and open circles represent measurements with the current perpendicular to and along the c -axis, respectively, with the residual resistivities $\rho_0^\perp = 6.78 \mu\Omega \text{ cm}$ and $\rho_0^\parallel = 6.14 \mu\Omega \text{ cm}$ having been subtracted. The solid curve is the sum of the electron-magnon ρ_{mag} and electron-phonon ρ_{ph} resistivities, whereas the dashed curve is the calculated electron-magnon resistivity ρ_{mag} alone.

The inset is a low-temperature blow-up of the same results (Andersen and Smith 1979).

the isotropic model it is equal to k_F^4/m^2). There is also arbitrariness in describing phonon scattering by means of eqs. (7.26) and (4.63), because $\bar{\tau}_F$ includes k_F , the sound velocity s and the constant Ξ . All of these parameters, however, change the scale of only the ordinates of the $1/\tau_{\text{mag}}$ and $1/\tau_{\text{ph}}$ curves.

It is from this point of view that the experimental results from fig. 15.5 are to be appraised. By means of a reasonable choice of the parameters, it proved possible to achieve excellent agreement between theory and the experimental data. But no one has succeeded as yet in directly confirming the existence of the dependence $1/\tau \propto \exp(-\Delta/T)$.

15.3. Magnetic impurities

Let us consider a semiconductor having a certain amount of magnetic atoms as impurities. An example is Mn, substituting for Cd in the semiconductor CdTe and producing the alloy $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$. Both Mn and Cd have the same number of valence s -electrons. Therefore, the most important result of the replacement of Cd by Mn is the occurrence of a half-filled $3d^5$ shell with $L = 0$ and $S = 5/2$ in place of the filled $4d^{10}$ shell with zero angular momenta S and L . Alloys of this type are called semimagnetic semiconductors [see references given by Dobrovolska et al. (1981)].

In scattering by magnetic impurities in a nonmagnetic crystal, not only the spin orientations of the impurities are random, but their arrangement as well. Hence the perturbation should be written in the form

$$\mathcal{H}(\mathbf{r}, t) = U(\mathbf{r}) + \mathbf{M}(\mathbf{r}, t) \cdot \mathbf{s}. \quad (15.56)$$

Here

$$U(\mathbf{r}) = \sum_{\alpha} v(\mathbf{r} - \mathbf{R}_{\alpha}) \quad (15.57)$$

is a random potential of the impurities; $v(\mathbf{r})$ is the effective potential of a single impurity, replacing the operator Q in Hamiltonian (15.9), and \mathbf{R}_{α} are the positions of the impurities. Then

$$\mathbf{M}(\mathbf{r}, t) = \sum_{\alpha} \mathcal{J}(\mathbf{r} - \mathbf{R}_{\alpha}) \mathbf{S}_{\alpha}(t) \quad (15.58)$$

is a random “magnetization” (expressed in energy units), set up by the impurities. This magnetization fluctuates with time due to the fluctuations in the directions of the spins of the impurities.

Let us make use of eq. (2.119) to calculate the scattering probability. Here, as mentioned in sect. 2.6, the average $\langle \mathcal{H} \rangle$ need not be eliminated. In considering the transition $\sigma \mathbf{k} \rightarrow \sigma' \mathbf{k}'$, $\mathcal{H}(\mathbf{r}, t)$ in eq. (2.119) is to be understood as the matrix element $\mathcal{H}_{\sigma' \sigma}(\mathbf{r}, t)$ of perturbation (15.56) calculated with the spin functions of a conduction electron. We choose the quantization axis z of electron spin along the average magnetization $\langle \mathbf{M}(\mathbf{r}, t) \rangle = \langle \mathbf{M} \rangle$. Then, for scattering without spin-flip,

$$\begin{aligned} \mathcal{H}_{\sigma \sigma}(\mathbf{r}, t) &= U(\mathbf{r}) + M_z(\mathbf{r}, t) \langle \sigma | s_z | \sigma \rangle \\ &= U(\mathbf{r}) \pm \frac{1}{2} M_z(\mathbf{r}, t), \end{aligned} \quad (15.59)$$

where the plus corresponds to $\sigma = \uparrow$ and the minus to $\sigma = \downarrow$. For spin-flip scattering

$$\mathcal{H}_{\sigma' \sigma}(\mathbf{r}, t) = \mathbf{M}(\mathbf{r}, t) \cdot \langle \sigma' | \mathbf{s} | \sigma \rangle \quad (\sigma' \neq \sigma), \quad (15.60)$$

which includes only the transverse (x, y) components of the vectors \mathbf{M} and \mathbf{s} .

Spin-flip scattering of an electron is feasible only as the result of fluctuations in magnetization, and, by complete analogy with eq. (15.37), we obtain

$$\begin{aligned} W_{\uparrow \mathbf{k} \rightarrow \downarrow \mathbf{k}'} &= \frac{1}{L^3} \frac{1}{4\hbar^2} \langle M^- M^+ \rangle_{q\omega}, \\ W_{\downarrow \mathbf{k} \rightarrow \uparrow \mathbf{k}'} &= \frac{1}{L^3} \frac{1}{4\hbar^2} \langle M^+ M^- \rangle_{q\omega}. \end{aligned} \quad (15.61)$$

In general this scattering is inelastic.

Scattering without spin-flip is determined by the correlator

$$\begin{aligned} & \langle [U(\mathbf{r}) \pm \frac{1}{2}M_z(\mathbf{r}, t)] [U(\mathbf{r}') \pm \frac{1}{2}M_z(\mathbf{r}', t')] \rangle \\ &= \langle U(\mathbf{r}) U(\mathbf{r}') \rangle \pm \frac{1}{2} [\langle U(\mathbf{r}) M_z(\mathbf{r}', t') \rangle + \langle M_z(\mathbf{r}, t) U(\mathbf{r}') \rangle] \\ & \quad + \frac{1}{4} \langle M_z(\mathbf{r}, t) M_z(\mathbf{r}', t') \rangle. \end{aligned} \quad (15.62)$$

Interference terms can first be averaged over time, after which they are independent of time. Therefore, not only is the scattering due to fluctuations in the potential elastic, but that due to interference of these fluctuations with those of the magnetization is also elastic. This part of the scattering has the probability

$$W'_{\sigma k \rightarrow \sigma k'} = \frac{1}{L^3} \frac{1}{4\hbar^3} 2\pi\delta(\omega) [\langle UU \rangle_q \pm \frac{1}{2} (\langle UM_z \rangle_q + \langle M_z U \rangle_q)]. \quad (15.63)$$

which depends upon the spin orientation; the plus refers to $\sigma = \uparrow$, and the minus to $\sigma = \downarrow$. In calculating the averaged probability given by eq. (15.36), the interference term cancels out. Magnetization fluctuations make their contribution to scattering without spin-flip:

$$W''_{\sigma k \rightarrow \sigma k'} = \frac{1}{L^3} \frac{1}{4\hbar^2} \langle M_z M_z \rangle_{q\omega}, \quad (15.64)$$

which is independent of spin orientation. In general, this scattering is inelastic.

In spin-flip scattering the electron can change its energy both at the expense of the spin energy of the atoms in the external magnetic field and of the energy of their interaction (of the dipole-dipole type). Only the second possibility remains in scattering without spin-flip.

At sufficiently low densities, the impurities interact only very weakly and almost always form a paramagnetic system. The spins at the various lattice sites do not correlate. Therefore, in calculating the correlators, approximation (2.125) of randomly arranged potentials can be applied, generalizing this relationship for the case of quantities that depend, not only on \mathbf{r} , but on t as well.

Thus, for example,

$$\begin{aligned} \langle M^i(0, 0) M^j(\mathbf{r}, t) \rangle &= N \int_{-\infty}^{\infty} dt' \int d^3r' \mathcal{J}(\mathbf{r}') S^i(t') \\ & \quad \times \mathcal{J}(\mathbf{r}' + \mathbf{r}) S^j(t' + t). \end{aligned} \quad (15.65)$$

Since the spin components are random functions of time, the integral with respect to t' can be dealt with as averaging, and we can write

$$\langle M^i(0, 0) M^j(\mathbf{r}, t) \rangle = N \langle S^i(0) S^j(t) \rangle \int d^3r' \mathcal{J}(\mathbf{r}') \mathcal{J}(\mathbf{r}' + \mathbf{r}). \quad (15.66)$$

It follows that

$$\langle M^i M^j \rangle_{q\omega} = N \langle S^i S^j \rangle_{\omega} |\mathcal{J}_q|^2, \quad (15.67)$$

where \mathcal{J}_q is the Fourier transform of $\mathcal{J}(\mathbf{r})$, determined according to eq. (9.20). In an analogous manner

$$\langle UM_z \rangle_q + \langle M_z U \rangle_q = 2\pi N \delta(\omega) \langle S_z \rangle (v_q \mathcal{J}_q^* + v_q^* \mathcal{J}_q). \quad (15.68)$$

The one-site averages appearing here can be calculated by making use of eq. (15.42). [Note that in this case the scattering given by eq. (15.64) becomes elastic.] This solves the problem of calculating the scattering probability in a paramagnetic system of impurity spins.

The scattering is elastic for $H = 0$, the interference term is absent, and the spin part of the scattering is the same as for scattering by a paramagnetic spin lattice. But in strong fields H the spatial disordering of the spins has an effect. The probability of elastic scattering (15.31) without spin-flip tends to zero for a lattice of noninteracting spins as $H \rightarrow \infty$. This becomes evident when eqs. (15.41) and (15.42) are used. Only the probability of spin-flip scattering, accompanied by the transfer of the energy $\hbar\omega = g\mu_B H \gg T$, remains finite; hence a thermal electron is actually not scattered. Meanwhile, in the same situation, but with a disordered spin arrangement, in addition to the strongly inelastic spin-flip scattering given by eq. (15.61), elastic scattering (15.64) without spin-flip also remains. This can be confirmed with the aid of eq. (15.67).

The scattering probability was calculated above for a free electron; the possibility of Landau quantization in an external field H , if there is one, and the actual band structure were not taken into consideration.

Since the effective mass of electrons in a semiconductor is appreciably smaller than the mass of a free electron, the cyclotron splitting $\hbar\Omega$ for the band electron is greater than the Zeeman splitting $g\mu_B H$ for an impurity atom. Hence, when the field H is switched on, Landau quantization for equilibrium electrons with $\varepsilon \sim T$ begins earlier than the alignment of the impurity spins. But this means that in fields H , before Landau quantization begins, scattering by spin impurities corresponds to small $g\mu_B H/T$ values, being, thereby, quasi-elastic.

As to the effect of actual band structure, it is not at all simple to take it into account within the framework of the general correlator method, even for semiconductors. The reason is that perturbation (15.56) is not smooth, and the effective-mass method cannot be applied. The band structure can be taken into account in a comparatively simple way for a random distribution of the scattering centers, when they scatter independently. It is obvious that in this case \mathcal{J}_q and v_q , which are the matrix elements with plane waves of the $\mathbf{k} \rightarrow \mathbf{k}'$ transition, should be replaced by matrix elements (15.27) and by $v_{\mathbf{k},\mathbf{k}'}$, defined in a similar manner. The expansion of the Bloch factors $u_{\mathbf{k}}$ in terms of the

basis functions at $\mathbf{k} = \mathbf{k}_0$ [see eq. (1.45)] is known for semiconductors. This enables integrals of the type of $\mathcal{J}_{\mathbf{k}, \mathbf{k}'}$ to be reduced to several constants, which are integrals calculated with the basis functions. Thus, for instance, only two constants, $\langle s | \mathcal{J} | s \rangle$ and $\langle p | \mathcal{J} | p \rangle$, remain in the Kane model (see sect. 1.3.4). In many cases these constants can be found by independent magneto-optical experiments because they determine the change of the band structure given by eq. (15.24) in a magnetic field, in which $\langle S_z \rangle$ becomes nonzero.

The momentum relaxation time in the Kane model for the conduction band in semiconductors of the InSb and HgTe types was calculated by Kossut (1975). Though semimagnetic semiconductors are being quite actively investigated, to date there are evidently no experiments in which spin scattering is clearly manifested. Probably it is masked by cruder effects: the change of the electron band structure owing to the exchange interaction, and the dependence of the g -factor on the field H and on the temperature T .

The theory of scattering by magnetic impurities in metals is being devised in a completely analogous manner (Fischer 1983). Many experimental data are available for metals, but, in this case, comparison with the theory discussed above is complicated by the Kondo effect. As has already been shown in sect. 2.6, the application of the method of correlators is equivalent to the first-order of the Born approximation. But, as was demonstrated by Kondo (1964), an important correction appears to the scattering probability for a degenerate system of conduction electrons in second-order Born approximation. As $T \rightarrow 0$ this correction increases as $\ln \mathcal{J}/T$. This indicates that the Born approximation is inapplicable and that it is necessary, in principle, to devise a more complex theory. These problems, however, are outside the scope of the visualizable physical considerations on which the present book is based.

At high impurity concentrations, there is a probability of forming clusters (pairs, triplets, etc.) of magnetic atoms located in adjacent unit cells. The spins of such impurities strongly interact, combining into the total spin of the cluster. Therefore, a cluster scatters differently from isolated impurities. The probability of scattering by a pair of magnetic atoms has been calculated by van Peski-Tinbergen and Dekker (1963) and by Matho and Beal-Monod

the electron scattering $\mathbf{k} \rightarrow \mathbf{k}'$ is asymmetrical with respect to the reflection of the vector \mathbf{k}' from a plane passing through \mathbf{k} and \mathbf{h} . In other words

$$W_{\mathbf{k} \rightarrow \mathbf{k}'} \neq W_{\mathbf{k} \rightarrow \tilde{\mathbf{k}}'}, \quad (15.69)$$

where $\tilde{\mathbf{k}}'$ is the vector \mathbf{k}' reflected from the plane mentioned above. Scattering with this probability is said to be "skew" (Fert 1973).

For the simplest case the probability of elastic skew scattering can be represented as follows:

$$W_{\mathbf{k} \rightarrow \mathbf{k}'} = [w(\varepsilon, \theta) + \bar{w}(\varepsilon, \theta) \mathbf{h}(\mathbf{n} \times \mathbf{n}')] \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}), \quad (15.70)$$

where θ is the scattering angle, ε is the energy of the electron being scattered, and \mathbf{n} and \mathbf{n}' are unit vectors along \mathbf{k} and \mathbf{k}' .

The principle of detailed balance, eq. (2.11), is not satisfied in such scattering. This means that for the scattering of a spinless particle by a spinless system, the skew transition probability can be obtained only in an approximation of a higher order than the Born approximation, and only in the case when the scattering system has no center of symmetry (Smit 1958, Luttinger 1958).

15.4.1. Spin-aligned band electrons

We shall now discuss the elastic scattering of electrons, whose spins are aligned along the z -axis, by a center having spherical symmetry, taking into account the spin-orbit interaction in the field of the center. This corresponds to Hamiltonian (15.9) with

$$Q = U(\mathbf{r}), \quad \mathbf{R} = -i(\hbar/2m^2c^2)[\nabla U(\mathbf{r}) \times \nabla], \quad (15.71)$$

where $U(\mathbf{r})$ is the field of the center.

In order to conceive of the nature of the scattering symmetry, we shall first discuss scattering in the (x, y) -plane, with the initial wavevector \mathbf{k} along $-x$. After applying the results of sect. 2.3, it can be readily shown that if \mathbf{k}' lies in the (x, y) -plane, the matrix of the scattering amplitude is

$$f = A(\theta) - 2\eta B(\theta) s_z, \quad \eta \equiv \text{sign } n'_y. \quad (15.72)$$

This matrix is diagonal and the spin orientation is conserved in scattering. Therefore, the scalar scattering amplitude is

$$f = A(\theta) \mp \eta B(\theta), \quad (15.73)$$

where the plus and minus correspond to electrons with spin up and with spin down. The scattering cross section in the (x, y) -plane is of the form

$$\sigma = |f|^2 = \sigma_0 \mp \eta \sigma_1, \quad \sigma_0 = |A|^2 + |B|^2, \quad \sigma_1 = AB^* + BA^*. \quad (15.74)$$

When the vector \mathbf{k} is reflected from the (x, z) -plane the sign of η is reversed so that the electrons of each polarization are scattered asymmetrically with

respect to this plane. If $\sigma_1 > 0$, electrons \uparrow are scattered mainly to the left, and electrons \downarrow mainly to the right. After averaging the cross section in eq. (15.74) over the spin orientations, we find that the average cross section for scattering in the (x, y) -plane is

$$\bar{\sigma} = w_{\uparrow} \sigma_{\uparrow} + w_{\downarrow} \sigma_{\downarrow} = \sigma_0 - \eta \rho_s \sigma_1, \tag{15.75}$$

where $w_{\uparrow, \downarrow}$ is the probability that the spin is either up or down, and $\rho_s = w_{\uparrow} - w_{\downarrow}$ is the degree of spin orientation (13.69). Thus, if the electron spins are polarized the average scattering cross section in the (x, y) -plane is asymmetrical.

When \mathbf{k} and \mathbf{k}' do not lie in the (x, y) -plane, spin-flip is possible in scattering. In this case $\bar{\sigma}_{\mathbf{k} \rightarrow \mathbf{k}'}$ is the sum over the final spin orientations and the average over the initial spin orientations. After making use of the well-known properties of the Pauli matrix, we can readily verify that

$$\begin{aligned} \bar{\sigma}_{\mathbf{k} \rightarrow \mathbf{k}'} &= \text{Tr}\{wff^\dagger\} \\ &= \sigma_0(\theta) + 2\langle s \rangle \nu_{\mathbf{k}\mathbf{k}'} \sigma_1(\theta). \end{aligned} \tag{15.76}$$

Here the dagger denotes the Hermitian conjugate of the spin matrices, w is the density spin matrix which, in our case, is

$$w = \begin{vmatrix} w_{\uparrow} & 0 \\ 0 & w_{\downarrow} \end{vmatrix}, \tag{15.77}$$

$\nu_{\mathbf{k}\mathbf{k}'}$ is the unit vector along $\mathbf{k} \times \mathbf{k}'$, and the average value of the spin,

$$\langle s \rangle = \text{Tr}\{ws\}, \tag{15.78}$$

is directed, in our case, along z and equals $\langle s_z \rangle = \frac{1}{2} \rho_s$.

Thus, in the scattering of electrons with polarized spins, the spin-averaged scattering probability is skewed in a way similar to eq. (15.70), with the “degree of skewness” proportional to the degree of spin polarization.

Note that scattering asymmetry vanishes if σ is calculated in the Born approximation. In this approximation, as is evident from eqs. (15.17) and (15.18), we have

$$f_{\mathbf{k} \rightarrow \mathbf{k}'} = f_{\mathbf{k}' \rightarrow \mathbf{k}}^\dagger. \tag{15.79}$$

The angle θ does not change when \mathbf{k} and \mathbf{k}' are interchanged, but the sign of the vector $\nu_{\mathbf{k}\mathbf{k}'}$ is reversed. Hence, in the Born approximation,

$$A^*(\theta) = A(\theta), \quad B^*(\theta) = -B(\theta), \tag{15.80}$$

so that the asymmetric term in eq. (15.74) vanishes. Scattering also ceases to be of the skew type when the spin-orbit interaction is neglected because, in this case, $B = 0$.

15.4.2. Magnetic atoms with aligned spins

The scattering of a conduction electron by a magnetic impurity is determined by a Hamiltonian of the type of eq. (15.9), in which Q and \mathbf{R} are to be understood to be the difference between the corresponding values for an impurity atom and for an atom of the host metal. The scattering amplitude for the $\mathbf{k} \rightarrow \mathbf{k}'$ transition is of the form of eq. (15.16). If the electron wavelength is large compared to the inner-shell radius of the impurity atom, i.e. if $ka^* \ll 1$, the quantities $A_{\mathbf{k}\mathbf{k}'}$, and $\mathbf{B}_{\mathbf{k}\mathbf{k}'}$, appearing in the corresponding equation, can be expanded into a power series in terms of \mathbf{k} and \mathbf{k}' . For simplicity we assume that the inner d- or f-shell is characterized only by the spin \mathbf{S} , and that the scattering center has spherical symmetry and a center of symmetry. There is no difficulty, in this case, in constructing the required scalars for $A_{\mathbf{k}\mathbf{k}'}$ and vectors for $\mathbf{B}_{\mathbf{k}\mathbf{k}'}$ from the components of the spin \mathbf{S} and the wavevectors \mathbf{k} and \mathbf{k}' . Since \mathbf{S} is a pseudovector, the terms of the expansion with odd powers of the wavevectors are forbidden by the center of symmetry. We limit the expansion to terms of up to second order in \mathbf{k} and \mathbf{k}' . Then the possible scalars for A are

$$1; \quad k^2, \mathbf{k}\mathbf{k}', (\mathbf{k} \times \mathbf{k}')\mathbf{S}, \dots \quad (15.81)$$

(the dotted line denotes invariants obtained by the interchange of \mathbf{k} and \mathbf{k}'). The possible vectors for \mathbf{B} are

$$\mathbf{S}; \quad \mathbf{k} \times \mathbf{k}', \mathbf{S}k^2, \mathbf{S}(\mathbf{k}\mathbf{k}'), \mathbf{k}(\mathbf{S}\mathbf{k}), \mathbf{k}(\mathbf{S}\mathbf{k}'), \dots \quad (15.82)$$

Only invariants that include \mathbf{S} to a power not higher than the first are given here. These are the only kind that exist when $S = \frac{1}{2}$. If the spin of the impurity is greater than $\frac{1}{2}$, invariants exist with higher powers of \mathbf{S} , but we shall not discuss them.

Under various conditions one of the various given invariants (or more complex ones, with higher powers of \mathbf{k} and \mathbf{S}) may make a contribution to the scattering asymmetry. As an example let us consider the scattering amplitude in the form

$$f = a + 2b\mathbf{S}\mathbf{s} + 2c\kappa\mathbf{s}, \quad \kappa \equiv \mathbf{k} \times \mathbf{k}'. \quad (15.83)$$

The first term results from the short-range potential of the impurity, the second from the exchange interaction of the electron with the inner magnetic shell, and the third term is due to the spin-orbit interaction of the electron in the field of the impurity.

In order to investigate the scattering asymmetry, we first assume that the impurity spins \mathbf{S} and the electron spins \mathbf{s} have no components transverse to the specified z -axis. Then, for scattering in the (x, y) -plane, the matrix of the scattering amplitude is

$$f = a + 2bS_z s_z + 2c\kappa_x s_x + 2c\kappa_y s_y. \quad (15.84)$$

No spin-flip occurs in such scattering, so that the scalar scattering amplitude for \uparrow and \downarrow electrons is

$$f = a \pm bS_z \pm c\kappa_z. \quad (15.85)$$

The corresponding cross sections are

$$\begin{aligned} \sigma = |f|^2 = & |a|^2 + |b|^2 S_z^2 + |c|^2 \kappa_z^2 \pm (ab^* + ba^*) S_z \pm (ac^* + ca^*) \kappa_z \\ & + (bc^* + cb^*) S_z \kappa_z. \end{aligned} \quad (15.86)$$

The scattering asymmetry is determined by the last two terms. The first of these terms provides for asymmetry that is opposite for electrons with different spin orientations, and the second term, for asymmetry that is the same for different spin orientations. These terms appear as a result of the interference of spin-orbit scattering with potential and exchange scattering. The fourth term in eq. (15.86), arising from the interference of potential scattering with exchange scattering, provides for symmetric scattering that differs for \uparrow and \downarrow electrons. Next we average cross section (15.86) over the orientations of the electron spins and the projections of the impurity spins. Then we obtain

$$\bar{\sigma} = \sigma_0 + \sigma', \quad (15.87)$$

in which the symmetrical part of the cross section is

$$\sigma_0 = |a|^2 + |b|^2 \langle S_z^2 \rangle + |c|^2 \kappa_z^2 + \rho_s \langle S_z \rangle (ab^* + ba^*), \quad (15.88)$$

and the asymmetrical part is

$$\sigma' = [\rho_s (ac^* + ca^*) + S_z (bc^* + cb^*)] \kappa_z. \quad (15.89)$$

The contribution to σ' , proportional to ρ_s is of the same nature as σ_1 in eqs. (15.74). A new contribution is that due to the polarization of the impurity spins. This contribution is independent of the degree of band electron spin polarization.

If we make use of relation (15.76) between $\bar{\sigma}$ and f , we shall encounter no difficulty in calculating the cross section $\bar{\sigma}$ even for an arbitrary direction of \mathbf{k} and \mathbf{k}' , rejecting, in addition, the artificial condition that the spins have no transverse components. Thus, for unpolarized band electrons,

$$\bar{\sigma} = [|a|^2 + |b|^2 S(S+1) + |c|^2 \kappa^2] + (bc^* + cb^*) \langle S \rangle \kappa. \quad (15.90)$$

In the Born approximation it follows from eq. (15.79) that the constants a and b are real, whereas c is purely imaginary, so that in this case as well, the scattering can be of the skew type only beyond the Born approximation.

15.4.3. Extraordinary Hall effect

In skew scattering, an electric field \mathbf{E} , perpendicular to \mathbf{h} , leads to a transverse current event for an isotropic band. This current can be readily calculated if

we assume that in eq. (15.70) the asymmetric part of the scattering is small compared to the symmetric part. When $\bar{w} = 0$ the nonequilibrium part of the distribution function [see eq. (7.1)] is

$$\delta f_{\mathbf{k}} = \left(-\frac{\partial f_T}{\partial \varepsilon} \right) e \mathbf{E} \mathbf{v}_{\mathbf{k}} \tau_1(\varepsilon), \quad (15.91)$$

where $\tau_1(\varepsilon)$ is the transport time corresponding to the term w . Taking \bar{w} into account as a small perturbation leads to an additional term in the nonequilibrium part of the distribution function, namely

$$\delta f'_{\mathbf{k}} = \frac{1}{2} \frac{\tau_1(\varepsilon)}{\bar{\tau}_\perp(\varepsilon)} \left(-\frac{\partial f_T}{\partial \varepsilon} \right) (\mathbf{h} \times e \mathbf{E}) \mathbf{v}_{\mathbf{k}} \tau_1(\varepsilon), \quad (15.92)$$

where $\bar{\tau}_\perp(\varepsilon)$ is the “spreading time” given by eq. (2.70), corresponding to the term \bar{w} . Note that \bar{w} , in contrast to w , is not necessarily positive; hence $\bar{\tau}_\perp$ can have either sign. A positive \bar{w} corresponds to predominant scattering “to the left”: if \mathbf{h} is along z and an electron ($e < 0$) is incident from the side of the x -axis (i.e. \mathbf{k} is along $-x$), the electron is scattered mainly toward $-y$. In this case the main current, associated with $\delta f_{\mathbf{k}}$, is along $+x$, and the supplementary current, associated with $\delta f'_{\mathbf{k}}$, is along $+y$. We readily see that

$$\sigma_{xx} = \frac{ne^2}{m} \langle\langle \tau_1 \rangle\rangle \equiv \sigma_0, \quad \sigma_{yx}^E = \frac{ne^2}{m} \left\langle \left\langle \frac{\tau_1^2}{2\bar{\tau}_\perp} \right\rangle \right\rangle. \quad (15.93)$$

The angular brackets denote averaging according to eq. (7.16). The superscript E of σ_{yx} indicates that this is an extraordinary transverse conductivity, arising from the fact that the scattering has a skew component. In comparison to the longitudinal conductivity, the transverse conductivity has the additional small factor $\tau_1/\bar{\tau}_\perp \sim \bar{w}/w$. The sign of this transverse conductivity depends upon the sign of the scattering asymmetry. Predominant electron scattering to the left leads to the same effect as a magnetic field \mathbf{H} along the direction of \mathbf{h} . If the magnetic field is weak, i.e. $\Omega\tau_1 \ll 1$, its contribution to σ_{yx} and that of skew scattering are additive, with the former equal to

$$\sigma_{yx}^H = \frac{ne^2}{m} \Omega \langle\langle \tau_1^2 \rangle\rangle, \quad (15.94)$$

so that the total transverse conductivity is

$$\sigma_{yx} = \sigma_{yx}^E + \sigma_{yx}^H. \quad (15.95)$$

But since

$$\sigma_{yx}^E/\sigma_{yx}^H \sim (\Omega\bar{\tau}_\perp)^{-1}, \quad (15.96)$$

the extraordinary Hall effect can be greater than the ordinary effect, notwithstanding the small value of \bar{w}/w .

It follows from the aforesaid that skew scattering should lead to the appearance of the extraordinary Hall effect, which is added to the ordinary Hall effect. The latter arises in crossed fields $\mathbf{H} \perp \mathbf{E}$ as a result of carrier drift across both fields. From an experimental point of view, the problem of observing the extraordinary Hall effect consists in separating the contribution of σ_{yx}^E from the measured Hall coefficient

$$R = \rho_{xy}/H \sim \sigma_{yx}/\sigma_0^2 H. \quad (15.97)$$

Let us consider, for example, the alloys of the noble metals with the rare earths. At 1 at% of the rare earth, the residual resistivity of such an alloy is of the order of $10 \mu\Omega \text{ cm}$. Therefore, the rate of electron scattering in the alloy by rare-earth atoms, which are magnetic impurities, is about $10^{13} - 10^{14} \text{ s}^{-1}$. In a 10 kOe field, the value of $\Omega\tau_1$ is approximately 10^{-2} , i.e. $\Omega\tau_1 \ll 1$, so that eqs.

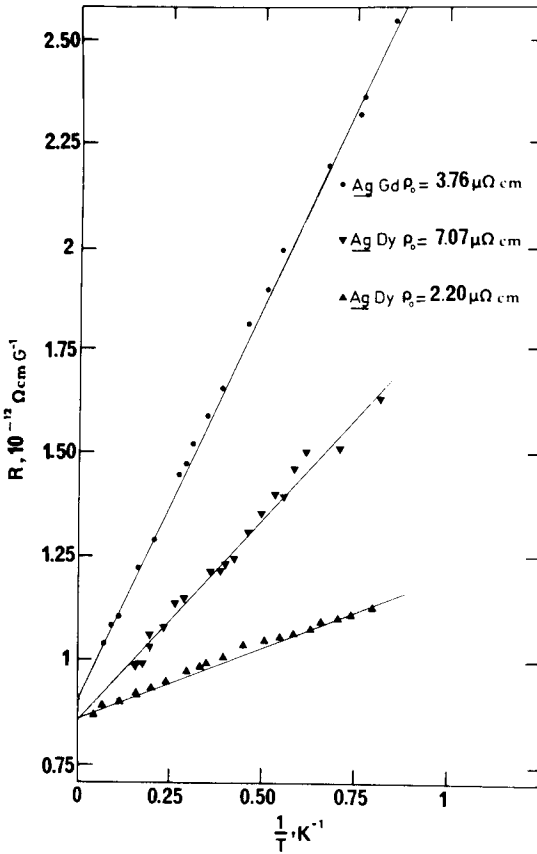


Fig. 15.6. Temperature dependence of the limiting Hall coefficient extrapolated to zero-field for AgGd and AgDy alloys (Fert and Friederich 1976).

(15.93)–(15.96) are applicable. The phonon scattering in these alloys is weaker than the impurity scattering right up to room temperature. Therefore, the ordinary Hall coefficient R^H is independent of temperature. This, exactly, is what enables the contribution of skew scattering to be separated out because it depends upon temperature (Fert and Friederich 1976). In fact, the skew scattering cross section σ' , according to eq. (15.90), is proportional to $\langle S \rangle$, i.e. to the average value of the magnetization. If the magnetic field is sufficiently weak, the magnetization satisfies Curie's law, i.e. $|\langle S \rangle| \propto H/T$ and $\sigma_{yx}^E \propto 1/T$. Shown in fig. 15.6 is the dependence, in silver-base alloys, of the limiting value of the Hall coefficient, i.e. its value as $H \rightarrow 0$, on the reciprocal T^{-1} of the temperature. The straight line obtained, intercepts the quantity R^H on the ordinate axis, and the quantity $R^E = R - R^H$ is the contribution of skew scattering. The different slopes of the lower two full lines in fig. 15.6 are due to the different concentrations N of dysprosium. By using the proportionality of the concentration N and the residual resistivity ρ_0 , we can see that $R^E \propto N$. This proportionality is the natural consequence of the fact that the rate of skew scattering is $1/\tau_{\perp} \propto N\sigma'$.

Finally, still another special feature of the extraordinary Hall effect, one that lends itself to experimental verification, follows from eq. (15.90). Since

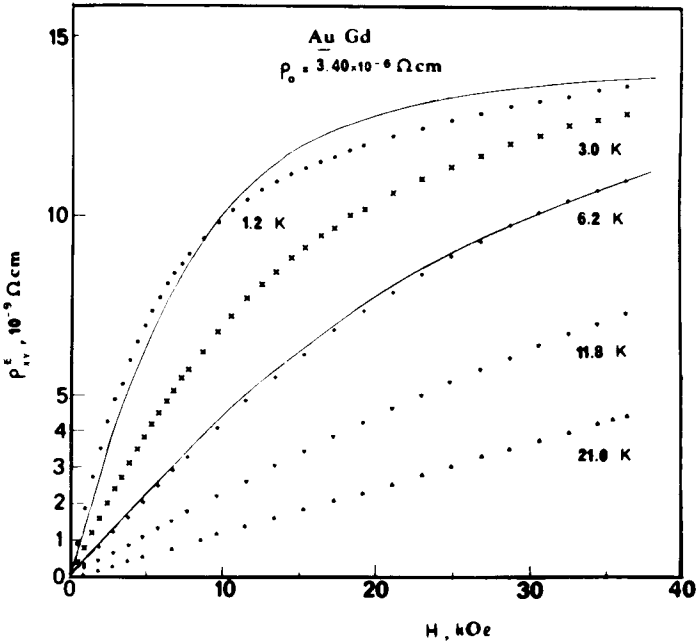


Fig. 15.7. Extraordinary Hall resistivity ρ_{xy}^E of an AuGd alloy versus the magnetic field at various temperatures. The solid lines represent the Brillouin functions (15.43) with $J = 7/2$ and $g = 2$ for $T = 6.2$ and 2 K (Fert and Friederich 1976).

the quantity $|\langle S \rangle|$ tends to saturation as the field H is increased, and the rate at which this occurs increases as T is lowered, the extraordinary Hall coefficient R^E should behave in the same way. Such behaviour of the quantity ρ_{xy}^E is demonstrated in fig. 15.7. Shown in this graph along with the experimental points are two Brillouin functions (15.43) for two temperatures, $T = 6.2$ K and 2 K, the functions corresponding to the magnetization curves for a system of impurity atoms. The curves are normalized in such a way that they approach the same limiting value in strong fields that the experimental curves do. Then the coefficients of σ' in eq. (15.90) is determined from the normalization constant. It is quite evident from the graphs in fig. 15.7 that

$$\bar{w}/w \sim \sigma_{yx}^E/\sigma_0 \approx \rho_{xy}^E/\rho_0 \lesssim 0.3 \times 10^{-2},$$

which justifies the perturbation calculation of the nonequilibrium parts given by eqs. (15.91) and (15.92) of the distribution function.

15.5. Electron spin relaxation in exchange interaction with holes

Adjoining the problems discussed in the present chapter is the problem on spin-flip of the electron in its interaction with holes. This process is described by a Hamiltonian of the type of eq. (15.14) though, as is clear from its derivation (Bir and Pikus 1974, §27), the meaning of the delta function in Hamiltonian (15.98) is not the same as in eq. (15.13). This section deals with the calculation of the spin-flip time $\tau_s(\mathbf{k})$ for a conduction electron scattered by an equilibrium distribution of heavy holes in a wide-gap semiconductor of the GaAs type (Bir et al. 1975).

15.5.1. Rate of spin-flip

The exchange interaction of an electron and a hole in the isotropic approximation is described by the Hamiltonian

$$\mathcal{H} = C\delta(\mathbf{r}_1 - \mathbf{r}_2)(\mathbf{J}\mathbf{s}). \quad (15.98)$$

Here the electron and hole are described in the effective mass approximation, with \mathbf{r}_1 and \mathbf{r}_2 being their coordinates and \mathbf{s} and \mathbf{J} their angular momenta ($s = \frac{1}{2}$ and $J = \frac{3}{2}$). These momenta are to be understood as matrices of (2×2) and (4×4) order, operating in the space of the basis functions of the corresponding band. Thus, the components J_x , J_y and J_z are matrices, determined in eq. (1.50) and operating in the basis $p_{3/2}$ of the hole band ($m = \pm \frac{3}{2}, \pm \frac{1}{2}$), and the components s_x , s_y and s_z are Pauli matrices (to an accuracy within a factor of $\frac{1}{2}$), operating in the basis $s_{1/2}$ of the conduction band ($m = \pm \frac{1}{2}$). The constant C in eq. (15.98) can, in principle, be de-

terminated experimentally from the value of the exchange splitting Δ between the states of an exciton with $K=1$ and $K=2$, where $\mathbf{K}=\mathbf{J}+\mathbf{s}$ is the total angular momentum of the exciton:

$$C = \frac{1}{2}\pi a_B^3 \Delta, \quad (15.99)$$

where a_B is the Bohr radius of the exciton.

The matrix element of the transition induced by perturbation (15.98) is to be calculated with the following wave functions:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{L^{3/2}} e^{i\mathbf{k}\mathbf{r}_1} A_\sigma(\mathbf{k}) \frac{1}{L^{3/2}} e^{i\mathbf{p}\mathbf{r}_2} A_\mu(\mathbf{p}) S_{\mathbf{v}_k - \mathbf{v}_p}. \quad (15.100)$$

Here \mathbf{k} and \mathbf{p} are the wavevectors of the electron and hole, A_σ and A_μ are column vectors determining the wave functions of free particles in accordance with the effective mass method (see sect. 1.2), and \mathbf{v}_k and \mathbf{v}_p are the velocities of the electron and hole. The subindex $\sigma = \uparrow, \downarrow$ denotes the projection of the electron spin onto a certain axis, and μ is the projection of the hole angular momentum onto \mathbf{p} . The Sommerfeld factor S takes into account the long-range nature of the Coulomb field, owing to which the wave function of the unbound (but interacting!) electron-hole pair differs from the wave function of two noninteracting particles. If the screening radius λ is large, i.e. $\lambda \gg a_B$, then

$$S_v = \frac{2\pi\eta}{1 - e^{-2\pi\eta}} \equiv S(\eta), \quad \eta = \left(\frac{mv^2}{2\varepsilon_B} \right)^{-1/2}, \quad (15.101)$$

where m is the reduced mass, v is the relative velocity, and ε_B is the Bohr energy of the exciton. If, however, $\lambda \ll a_B$, then $S_v = 1$.

On the basis of the aforesaid we can write the equation for the electron spin-flip time (for a Boltzmann gas of electrons). In the calculations we obtain the sum

$$\sum_{\mu, \mu' = \pm 3/2} \left| A_{\downarrow}^{\dagger}(\mathbf{k}') s A_{\uparrow}(\mathbf{k}) A_{\mu'}^{\dagger}(\mathbf{p}') J A_{\mu}(\mathbf{p}) \right|^2. \quad (15.102)$$

In a wide-gap semiconductor, the admixture of p -states in the conduction band can be neglected, and then A_σ is independent of \mathbf{k} ; this is evident from eq. (1.96). After using the explicit form of the Pauli matrices, this sum can be written as

$$\sum_{\mu, \mu' = \pm 3/2} \left| A_{\mu'}^{\dagger}(\mathbf{p}') \frac{1}{2}(J_x + iJ_y) A_{\mu}(\mathbf{p}) \right|^2 \equiv G_{\mathbf{p}, \mathbf{p}'}. \quad (15.103)$$

After introducing this notation we have

$$\begin{aligned}
 \frac{1}{\tau_s(\mathbf{k})} &= \sum_{\mathbf{k}'\mathbf{p}\mathbf{p}'} \frac{2\pi}{\hbar} \frac{C^2}{L^6} \delta_{\mathbf{k}+\mathbf{p},\mathbf{k}'+\mathbf{p}'} \delta(\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{p}'}) \\
 &\quad \times f_{\mathbf{p}}(1 - f_{\mathbf{p}'}) G_{\mathbf{p},\mathbf{p}'} S_{v_{\mathbf{k}} - v_{\mathbf{p}}} S_{v_{\mathbf{k}'} - v_{\mathbf{p}'}} \\
 &= \frac{2\pi}{\hbar} C^2 \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3p}{(2\pi)^3} \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}} + \varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{q}}) f_{\mathbf{p}}(1 - f_{\mathbf{p}+\mathbf{q}}) \\
 &\quad \times G_{\mathbf{p}',\mathbf{p}+\mathbf{q}} S_{v_{\mathbf{k}} - v_{\mathbf{p}}} S_{v_{\mathbf{k}-\mathbf{q}} - v_{\mathbf{p}+\mathbf{q}}}. \tag{15.104}
 \end{aligned}$$

The factor $G_{\mathbf{p},\mathbf{p}'}$ can be calculated using the column vector $A_{\mu}(\mathbf{p})$, given in sect. 1.3.3. If the split-off hole band is sufficiently far away and the one-band approximation can be used for the hole band, $G_{\mathbf{p},\mathbf{p}'}$ depends only on the directions \mathbf{p} and \mathbf{p}' (with respect to each other and to the z -axis).

To proceed we assume the electrons are light ($m_c \ll m_h$) and not too hot, i.e. $\varepsilon_k \ll (m_h/m_c)T$ for Maxwellian holes or $\varepsilon_k \ll (m_h/m_c)\varepsilon_F$ for Fermi holes. In addition, we shall disregard cold electrons with $\varepsilon_k \ll T$. Under these conditions, as is evident from the conservation laws, $q \sim k \ll p$. This enables us to write $G_{\mathbf{p},\mathbf{p}+\mathbf{q}} = G_{\mathbf{p},\mathbf{p}}$ and $\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{q}} = -v_{\mathbf{p}}\hbar\mathbf{q}$.

First we shall consider a Maxwellian gas of holes. Here the electrons are fast: $v_k \gg v_p$, and the scattering is quasi-elastic: $\hbar\omega \ll T \leq \varepsilon_k$ (where $\hbar\omega$ is the energy transfer). Hence the Sommerfeld factors in eq. (15.104) are equal and depend only on the initial energy ε_k . As a result

$$\frac{1}{\tau_s(\mathbf{k})} = \frac{2\pi}{\hbar} C^2 \bar{G} |S_{v_k}|^2 \left(\frac{1}{2}N\right) g(\varepsilon_k), \tag{15.105}$$

where \bar{G} is the average of $G_{\mathbf{p},\mathbf{p}}$ over the angles of \mathbf{p} , N is the hole density, $g(\varepsilon)$ is the density of states of the electron, and S_{v_k} is given by eq. (15.101) with $\eta = (\varepsilon_k/\varepsilon_B)^{-1/2}$, and ε_B is calculated with the mass m_c . After substituting eq. (15.99) and $\bar{G} = \frac{3}{4}$ into the preceding equation, we obtain

$$\frac{1}{\tau_s(\mathbf{k})} = \frac{1}{\bar{\tau}} \eta^{-1} S^2(\eta), \quad \frac{\hbar}{\bar{\tau}} \equiv \frac{3\pi}{64} N a_B^3 \frac{\Delta^2}{\varepsilon_B}. \tag{15.106}$$

The spin-flip time turns out to be independent of the orientation of \mathbf{k} with respect to z , and also independent of the hole temperature.

We turn now to a Fermi gas of holes. It proves convenient to consider two cases separately: “moderate temperatures”, when $T/\varepsilon_F \gg m_c/m_h$, and “low temperatures”, when the inequality is reversed.

Moderate temperatures. Here, as in a Maxwellian gas, the electrons are fast for all ε_k ; hence $v_k \gg v_F$, and the scattering is kinematically quasi-elastic: $\hbar\omega \ll \varepsilon_k$. But, in a Fermi gas, a comparison of $\hbar\omega$ with T , i.e. statistical quasi-elasticity

(see sect. 2.4), is also of importance. In estimating $\hbar\omega \sim qv_F$, it can be shown that $\hbar\omega \sim (\varepsilon_k/\bar{\varepsilon})^{1/2}$, where $\bar{\varepsilon} = (m_h/m_c)(T^2/\varepsilon_F) \gg T$. (Note that the meaning of the energy $\bar{\varepsilon}$ is close to that of the energy T^2/ms^2 , which separates the regions of induced and spontaneous scattering by acoustic phonons; see sect. 4.2.2.) For $\varepsilon_k \ll \bar{\varepsilon}$, the general equation, eq. (15.104), is simplified as follows:

$$\frac{1}{\tau_s(\mathbf{k})} = \frac{2\pi}{\hbar} C^2 \bar{G} |S_{v_k}|^2 \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3p}{(2\pi)^3} \times \delta(\varepsilon_k - \varepsilon_{k-q}) f_p (1 - f_p) G_{p,p}, \quad (15.107)$$

from which

$$\begin{aligned} \frac{1}{\tau_s(\mathbf{k})} &= \frac{2\pi}{\hbar} C^2 \bar{G} |S_{v_k}|^2 g(\varepsilon_k) T g_F \\ &= \frac{3}{2} \frac{1}{\bar{\tau}} \frac{T}{\varepsilon_F} \eta^{-1} S^2(\eta), \end{aligned} \quad (15.108)$$

where g_F is the density of states of the holes at the Fermi level. This expression differs from eq. (15.105) in that the total hole density has been replaced by the number of holes in a thermal layer of thickness T . For $\varepsilon_k \gg \bar{\varepsilon}$ we can put $T = 0$ in general equation (15.104). In this case, as is quite evident, we find a dependence of $\tau_s(\mathbf{k})$ on the orientation of \mathbf{k} with respect to z . We restrict ourselves to the calculation of the average over the orientations of \mathbf{k} . This averaging is equivalent to averaging over the directions of z , leading to the substitution of \bar{G} for $G_{p,p}$ in the integrand. After this the integral can be readily evaluated; holes in a layer of the thickness $\hbar kv_F$ are found to be relevant:

$$\left\langle \frac{1}{\tau_s(\mathbf{k})} \right\rangle = \frac{9}{2} \frac{1}{\bar{\tau}} \left(\frac{m_c}{m_h} \right)^{1/2} \left(\frac{\varepsilon_B}{\varepsilon_F} \right)^{1/2} \eta^{-2} S^2(\eta). \quad (15.109)$$

Low temperatures. In this case the electrons are fast for $\varepsilon_k \gg (m_c/m_h)\varepsilon_F$; hence $v_k \gg v_F$, and the scattering is dynamically quasi-elastic: $\hbar\omega \ll \varepsilon_k$, but statistically nonquasi-elastic: $\hbar\omega \gg T$. Consequently, the situation is the same as at moderate temperatures with $\varepsilon_k \gg \bar{\varepsilon}$, and eq. (15.109) is applicable. For $\varepsilon_k \ll (m_c/m_h)\varepsilon_F$, the electrons are slow: $v_k \ll v_F$. Therefore, the Sommerfeld factor, if it must be taken into account, is determined by the velocity v_F . We can write the scattering probability, averaged over the angles, as

$$\begin{aligned} \left\langle \frac{1}{\tau_s(\mathbf{k})} \right\rangle &= \frac{2\pi}{\hbar} C^2 \bar{G} |S_{v_F}|^2 \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3p}{(2\pi)^3} \int d\omega \delta(\varepsilon_k - \varepsilon_{k-q} - \hbar\omega) \\ &\times \delta(\omega - v_F q) f(\varepsilon_p) [1 - f(\varepsilon_p + \hbar\omega)]. \end{aligned} \quad (15.110)$$

We begin by averaging over the directions of \mathbf{p} :

$$\int \frac{d\mathbf{o}_p}{4\pi} \delta(\omega - \mathbf{v}_p \mathbf{q}) = \frac{1}{2v_F q} \Theta(\omega - v_F q), \quad (15.111)$$

where $\Theta(x)$ is a step function, and then integrate with respect to \mathbf{p} :

$$\int \frac{d^3 p}{(2\pi)^3} f(\varepsilon_p) [1 - f(\varepsilon_p + \hbar\omega)] = g_F \frac{\hbar\omega}{1 - e^{-\hbar\omega/T}}. \quad (15.112)$$

After noting that $\omega \ll v_F q$ in the region being considered, and returning to integration with respect to \mathbf{k}' , we have

$$\left\langle \frac{1}{\tau_s(\mathbf{k})} \right\rangle = C^2 \bar{G} |S_{v_F}|^2 \frac{m_h^2}{2\hbar^5} \int \frac{d^3 k'}{(2\pi)^3} \frac{\varepsilon_{k'} - \varepsilon_k}{|\mathbf{k}' - \mathbf{k}|} [e^{(\varepsilon_{k'} - \varepsilon_k)/T} - 1]^{-1}. \quad (15.113)$$

After going over to dimensionless variables in the integral with respect to \mathbf{k}' , we can transform the obtained expression into the following form:

$$\left\langle \frac{1}{\tau_s(\mathbf{k})} \right\rangle = \frac{\pi^2}{16} \frac{1}{\bar{\tau}} \left(\frac{T}{\varepsilon_F} \right)^{3/2} \left(\frac{T}{\varepsilon_B} \right)^{1/2} \left(\frac{m_h}{m_c} \right)^{1/2} |S_{v_F}|^2 \mathcal{X} \left(\frac{\varepsilon_k}{T} \right), \quad (15.114)$$

where

$$\mathcal{X}(x) = 1 + \frac{6}{\pi^2} x^2 \int_0^1 \frac{dz z^{1/2} (1-z)}{1 - e^{-x(1-z)}}, \quad (15.115)$$

and

$$\begin{aligned} \mathcal{X}(x) &\approx 1 + (4/\pi^2)x, & \text{for } x \ll 1, \\ &\approx (8/5\pi^2)x^2, & \text{for } x \gg 1. \end{aligned} \quad (15.116)$$

If the electron is scattered by a hole bound to an acceptor, the wave function given by eq. (15.100) should be replaced by the function

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{L^{3/2}} e^{i\mathbf{k}\mathbf{r}_1} A_a(\mathbf{k}) \Phi_\mu(\mathbf{r}_2), \quad (15.117)$$

where the column vector Φ is the wave function of a localized hole. The Sommerfeld factor $S = 1$ because, in the case being discussed, a free electron travels in the field of a neutral center. In the case of a spherically symmetric state Φ , the spin-flip time turns out to be close to that obtained for a Maxwellian gas of holes. For $\varepsilon_k \ll \varepsilon_B$, we have

$$\frac{1}{\tau_s(\mathbf{k})} = \frac{1}{\bar{\tau}_a} \eta^{-1/2}, \quad \frac{\hbar}{\bar{\tau}_a} = \frac{5\pi}{64} N_a a_B^3 \frac{\Delta^2}{\varepsilon_B}, \quad (15.118)$$

where N_a is the density of localized holes, i.e. neutral acceptors.

15.5.2. Spin relaxation in GaAs and GaSb

Described in sect. 13.6.2 were experiments conducted with photo-electrons having oriented spins; these experiments enabled the time τ_s to be measured directly [see eqs. (13.72) and (13.73)]. Systematic experiments for the investigation of the dependence of the time τ_s on temperature and on the doping in GaAs and GaSb crystals enabled Aronov et al. (1983) to specify clearly the range of temperatures and impurity densities in which the spin relaxation mechanism described in sect. 15.5.1 predominates.

Given as an example in fig. 15.8 are the dependences of the time τ_s on the density N of shallow acceptors of Zn in GaSb crystals. The arrow indicates the critical density N_c , above which the shallow acceptors are metallized, leading to the formation of a weakly degenerate gas of holes. Valid for this region is eq. (15.108). For $N < N_c$ the holes are distributed between the localized states on the acceptors and the free states. Hence the time τ_s should be characterized by the sum of expressions (15.106) and (15.118). As is evident from fig. 15.8, both regions have exactly the density dependences that were predicted by the equations of sect. 15.5.1. The dependence $\tau_s \propto N^{-1}$ is predicted, as well, according to eqs. (13.36) and (13.28), in spin-flip due to the spin-orbit interaction in the impurity field. But in this case the time τ_s exceeds the experimental values by two orders of magnitude.

The circles in fig. 15.9a indicate the results of measurement of the dependence of τ_s on T for $N < N_c$. The continuous curve was plotted from data obtained in calculations based on eqs. (15.106) and (15.118). Here the quantity

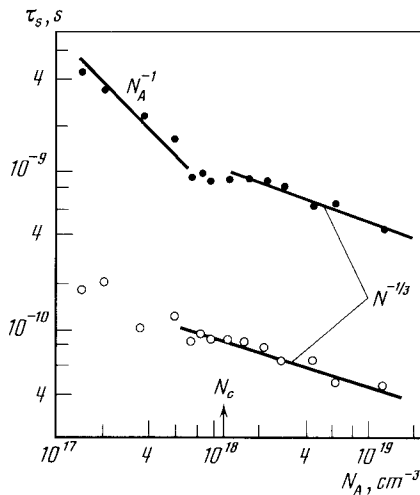


Fig. 15.8. Dependence of the time τ_s on the density N_A of shallow Zn acceptors in GaSb crystals at $T = 15$ K (solid circles) and 77 K (open circles) (Aronov et al. 1983).

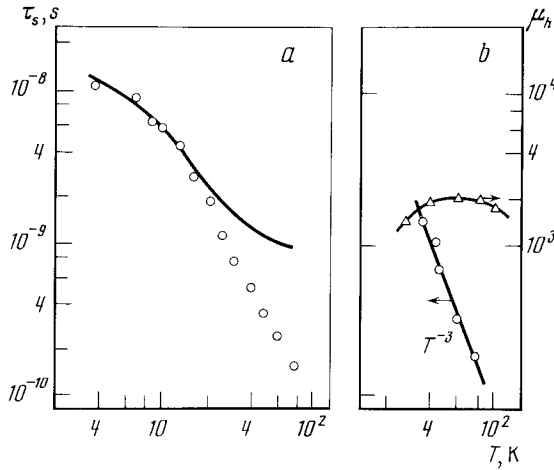


Fig. 15.9. Temperature dependence of the time τ_s in GaSb crystals with $N < N_c$. In (a) the open circles are the experimental data, and the solid curve is the theoretical relationship according to eqs. (15.106) and (15.118), with $N_A = 2.8 \times 10^{17} \text{ cm}^{-3}$; in (b) the open circles represent the quantities $\tau_s = [(1/\tau_s)_{\text{exp}} - (1/\tau_s)_{\text{calc}}]^{-1}$, taken from fig. 15.9a. The solid curve in fig. 15.9b is the theoretical relationship (13.55) calculated from data (triangles) on the temperature dependence of the hole mobility (Aronov et al. 1983).

$\bar{\tau}$, required for the calculations, was determined from similar measurements with $N > N_c$. Hence, in calculating this curve there were no free parameters. The fact that a difference exists between the calculated and experimental data indicates that a new scattering mechanism begins to operate as the tempera-

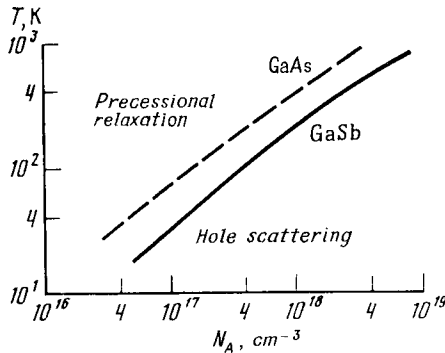


Fig. 15.10. Domains in the (T, N_A) plane in which the precessional spin relaxation mechanism and relaxation through electron-hole scattering predominate in GaAs and GaSb (Aronov et al. 1983).

ture is raised and that this mechanism leads to spin-flip with the scattering rate

$$1/\tau_s = (1/\tau_s)_{\text{exp}} - (1/\tau_s)_{\text{calc}} \quad (15.119)$$

The points in fig. 15.9b indicate the values of τ_s obtained by subtraction according to eq. (15.119). The straight line passing through these points was independently plotted. It represents the spin-flip time in accordance with the precessional mechanism, and was calculated by employing eq. (13.55), using independent measurements of the transport time τ_1 (these measurement data are also given in fig. 15.9b). The fact that the points coincide with the calculated curve indicates that in this crystal it is precisely the precessional mechanism that becomes predominant as the temperature is raised.

Figures 15.8 and 15.9 are examples illustrating how the experimental data were analyzed. The results of this analysis are summarized in fig. 15.10.

15.5.3. Effect of elastic scattering on spin relaxation

The electron spin-flip time calculations carried out above are based on the assumption that in the course of the interaction time, both the hole and electron are in quite definite states with definite wavevectors and projections of their angular momenta. This assumption is at the root of the concept of the probability of the process $k\sigma p\mu \rightarrow k'\sigma'p'\mu'$ (and at the basis of the kinetic equation in general). The interaction time t_{int} is a/v , where a is the dimension of the region of interaction and v is the relative velocity of the particles. The interaction distance a is determined by the momentum transfer $\hbar q$, so that $t_{\text{int}} \sim (qv)^{-1}$. Hence, the concept of the probability of an elementary event is valid if $qv \gg \tau^{-1}$, where τ is the relaxation time of the quantum parameters that specify the states of the colliding particles. This inequality is not satisfied if the holes are effectively scattered by some kind of imperfections, for instance, impurities, because such scattering destroys the hole states specified by the wavevector and the projection of the angular momentum. Therefore, the equations given above for $\tau_s(\mathbf{k})$ are valid only when $kv \gg (\tau_1^{-1})_h$ and $kv \gg (\tau_s^{-1})_h$, where $(\tau_1)_h$ is the momentum relaxation time and $(\tau_s)_h$ is the angular momentum relaxation time for holes. If even one of these two inequalities is not satisfied, the calculation of τ_s is extremely complicated (Bir et al. 1975), though semiquantitatively its result can be readily understood. Let us consider, for example, a Fermi gas of fast holes, when $v = v_F$. When $kv_F \gg (\tau_1^{-1})_h$, the holes pass ballistically through the interaction region without being scattered by imperfections, so that $t_{\text{int}} \sim a/v_F$. But if $kv_F \ll (\tau_1^{-1})_h$, the hole will be repeatedly scattered by imperfections as it passes through the region of interaction with an electron, and its motion will be of a diffusional type. As a result, $t_{\text{int}} \sim a^2/D$, where $D = \frac{1}{3}v_F^2(\tau_1)_h$ is the hole diffusion coefficient in scattering by imperfections. It is obvious that the spin-flip

probability is proportional to t_{int} . Consequently, if the inequality $kv_F \gg (\tau_1^{-1})_h$ is not satisfied and is replaced by the reverse inequality, the spin-flip probability given by eq. (15.114) should be multiplied by

$$\frac{a^2/D}{a/v_F} \sim \frac{(\tau_1^{-1})_h}{kv_F} \gg 1, \quad (15.120)$$

i.e. strong hole momentum relaxation increases the spin-flip probability of an electron scattered by these holes.

When the inequality $kv_F \gg (\tau_s^{-1})_h$ is not satisfied, a hole has a definite spin only during the short time $(\tau_s)_h$. Therefore, the estimate $t_{\text{int}} \sim (\tau_s)_h$ is valid, and, when $kv_F \ll (\tau_s^{-1})_h$, eq. (15.114) should be multiplied by

$$\frac{(\tau_s)_h}{a/v_F} \sim \frac{kv_F}{(\tau_s^{-1})_h} \ll 1, \quad (15.121)$$

i.e. strong hole spin relaxation reduces the electron spin-flip probability. Exact equations for the averaged spin-flip probabilities are given by Bir et al. (1975).