5.7 Conduction-electron interactions

As we have already discussed in Section 1.4, the conduction electrons in the rare earth metals act as the medium through which the coupling is established between the $4f$ electrons localized on the ions. In this section, we shall investigate this *RKKY* coupling in more detail, and consider its influence on both the *spin waves* in the ferromagnetic phase, and also on the *conduction electrons* themselves. The indirect-exchange interaction is first derived, and its effects in limiting the *lifetimes* of the spin waves and in *polarizing* the conduction electrons are deduced. The enhancement of the *effective mass* of the conduction electrons by the dynamical magnetic fluctuations is then calculated. Finally, the modification of the *electrical resistivity* by the exchange interaction is discussed, including the *scattering* of the conduction electrons by the spin-wave excitations, and the influence of the magnetic ordering on the conduction-electron band structure. For completeness, we include the effect of *magnetic superzones* in periodic structures in this section.

5.7.1 The indirect-exchange interaction

The starting point for our consideration of the indirect exchange, or RKKY coupling, of the localized moments is the Heisenberg–Dirac exchange between the $4f$ electrons and the conduction electrons. The $4f$-core electrons of the ion at site i are assumed to be described to a good approximation by non-overlapping atomic wavefunctions $\phi_{4f}(\mathbf{r} - \mathbf{R}_i)$.

We shall neglect the spin–orbit coupling of the conduction electrons, and assume their wavefunctions to be the Bloch functions

$$\psi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})\, e^{i\mathbf{k}\cdot\mathbf{r}} = \psi_{n\mathbf{k}}(\mathbf{r}-\mathbf{R}_i)\, e^{i\mathbf{k}\cdot\mathbf{R}_i}, \tag{5.7.1}$$

independent of the spin state σ. $u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r}-\mathbf{R}_i)$ has the periodicity of the lattice, and n is the band index. The Hamiltonian of the conduction electrons in *second quantization* is

$$\mathcal{H}_s = \sum_{n\mathbf{k}\sigma} \varepsilon_{n\mathbf{k}} c^+_{n\mathbf{k}\sigma} c_{n\mathbf{k}\sigma}, \tag{5.7.2}$$

where the index s is conventionally used for the conduction electrons even though, as we saw in Section 1.3, they have predominantly d character. $c^+_{n\mathbf{k}\uparrow}$ creates and $c_{n\mathbf{k}\uparrow}$ annihilates a spin-up electron in the band-state $(n\mathbf{k})$, and they are Fermi-operators which satisfy the *anticommutation relations*

$$\begin{aligned} \{c_{n\mathbf{k}\sigma}, c^+_{n'\mathbf{k}'\sigma'}\} &\equiv c_{n\mathbf{k}\sigma} c^+_{n'\mathbf{k}'\sigma'} + c^+_{n'\mathbf{k}'\sigma'} c_{n\mathbf{k}\sigma} = \delta_{nn'}\delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'} \\ \{c^+_{n\mathbf{k}\sigma}, c^+_{n'\mathbf{k}'\sigma'}\} &= \{c_{n\mathbf{k}\sigma}, c_{n'\mathbf{k}'\sigma'}\} = 0. \end{aligned} \tag{5.7.3}$$

An exposition of second quantization may be found, for example, in White (1983). The exchange interaction between a pair of electrons is $-2I\mathbf{s}_1\cdot\mathbf{s}_2$, where I is the exchange integral. If $\mathbf{s}_1$ is the spin of a $4f$ electron at site i, then the sum over all the $4f$ electrons at this site gives

$$\sum_{4f\ el.} -2I\mathbf{s}_1\cdot\mathbf{s}_2 = -2I\mathbf{S}_i\cdot\mathbf{s}_2 = -2I(g-1)\mathbf{J}_i\cdot\mathbf{s}_2,$$

where I is an average value of the exchange integral for the $4f$ electrons, and states other than those in the ground-state J-multiplet are neglected. The spin-density of the conduction electrons at $\mathbf{r}$ may be expressed in second-quantized form so that, for instance,

$$s_{2z}(\mathbf{r}) = \sum_{nn'}\sum_{\mathbf{k}\mathbf{k}'} \psi^*_{n'\mathbf{k}'}(\mathbf{r})\psi_{n\mathbf{k}}(\mathbf{r})\tfrac{1}{2}\big(c^+_{n'\mathbf{k}'\uparrow}c_{n\mathbf{k}\uparrow} - c^+_{n'\mathbf{k}'\downarrow}c_{n\mathbf{k}\downarrow}\big). \tag{5.7.4}$$

The *sf-exchange interaction* is determined by the following exchange integral:

$$\begin{aligned} \int d\mathbf{r}_1 d\mathbf{r}_2 \psi^*_{n'\mathbf{k}'}(\mathbf{r}_1)\phi^*_{4f}(\mathbf{r}_2-\mathbf{R}_i)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\psi_{n\mathbf{k}}(\mathbf{r}_2)\phi_{4f}(\mathbf{r}_1-\mathbf{R}_i) \\ = \frac{1}{N} I(n'\mathbf{k}', n\mathbf{k}) e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_i}, \end{aligned}$$

with

$$I(n'\mathbf{k}',n\mathbf{k}) = N\int d\mathbf{r}_1 d\mathbf{r}_2 \psi^*_{n'\mathbf{k}'}(\mathbf{r}_1)\phi^*_{4f}(\mathbf{r}_2)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\psi_{n\mathbf{k}}(\mathbf{r}_2)\phi_{4f}(\mathbf{r}_1), \tag{5.7.5}$$

where N is the number of rare earth ions. If there are several $4f$ electrons per ion, $I(n'\mathbf{k}',n\mathbf{k})$ should again be averaged over their wavefunctions. The Hamiltonian $\mathcal{H}_{sf}$, describing the exchange interaction between the conduction electrons and the $4f$ electrons, is then found to be

$$\begin{aligned}\mathcal{H}_{sf} = -\frac{1}{N}\sum_i\sum_{nn'}\sum_{\mathbf{k}\mathbf{k}'}&(g-1)I(n'\mathbf{k}',n\mathbf{k})e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_i}\\ &\times\big[(c^+_{n'\mathbf{k}'\uparrow}c_{n\mathbf{k}\uparrow}-c^+_{n'\mathbf{k}'\downarrow}c_{n\mathbf{k}\downarrow})J_{iz}+c^+_{n'\mathbf{k}'\uparrow}c_{n\mathbf{k}\downarrow}J_i^- + c^+_{n'\mathbf{k}'\downarrow}c_{n\mathbf{k}\uparrow}J_i^+\big],\end{aligned} \tag{5.7.6}$$

in second quantization.

In the ordered ferromagnetic phase, we may use the MF approximation, in which case

$$\mathcal{H}_{sf}(\mathrm{MF}) = -\sum_{nn'}\sum_{\mathbf{k}}(g-1)I(n'\mathbf{k},n\mathbf{k})(c^+_{n'\mathbf{k}\uparrow}c_{n\mathbf{k}\uparrow}-c^+_{n'\mathbf{k}\downarrow}c_{n\mathbf{k}\downarrow})\langle J_z\rangle. \tag{5.7.7}$$

This Hamiltonian gives rise to both diagonal and off-diagonal contributions to the energies of the conduction electrons. The diagonal energies are

$$\begin{aligned}\varepsilon_{n\mathbf{k}\uparrow} &= \varepsilon_{n\mathbf{k}} - \langle J_z\rangle(g-1)I(n\mathbf{k},n\mathbf{k})\\ \varepsilon_{n\mathbf{k}\downarrow} &= \varepsilon_{n\mathbf{k}} + \langle J_z\rangle(g-1)I(n\mathbf{k},n\mathbf{k}).\end{aligned} \tag{5.7.8}$$

Second-order perturbation theory then gives the energies of the band electrons as

$$\widetilde{\varepsilon}_{n\mathbf{k}\sigma} = \varepsilon_{n\mathbf{k}\sigma} + \langle J_z\rangle^2(g-1)^2\sum_{n'\neq n}\frac{|I(n'\mathbf{k},n\mathbf{k})|^2}{\varepsilon_{n\mathbf{k}}-\varepsilon_{n'\mathbf{k}}}. \tag{5.7.9}$$

This dependence of the energies of the perturbed band-electrons on their state of polarization implies that the electron gas itself develops a nonzero magnetization. In order to calculate this moment, we first note that (5.7.9) corresponds to a replacement of $\mathcal{H}_s + \mathcal{H}_{sf}(\mathrm{MF})$ by an effective Hamiltonian for the band electron,

$$\widetilde{\mathcal{H}}_s = \sum_{n\mathbf{k}\sigma}\widetilde{\varepsilon}_{n\mathbf{k}\sigma}\widetilde{c}^+_{n\mathbf{k}\sigma}\widetilde{c}_{n\mathbf{k}\sigma}, \tag{5.7.10}$$

where the new Fermi operators are determined in terms of the old by

$$\begin{aligned}c_{n\mathbf{k}\uparrow} &= \widetilde{c}_{n\mathbf{k}\uparrow} + \sum_{n'}U_{\mathbf{k}}(n,n')\widetilde{c}_{n'\mathbf{k}\uparrow}\\ c_{n\mathbf{k}\downarrow} &= \widetilde{c}_{n\mathbf{k}\downarrow} - \sum_{n'}U_{\mathbf{k}}(n,n')\widetilde{c}_{n'\mathbf{k}\downarrow},\end{aligned} \tag{5.7.11a}$$

to leading order. $U_{\mathbf{k}}(n,n) = 0$ and, for $n' \neq n$,

$$U_{\mathbf{k}}(n,n') = (g-1)\langle J_z\rangle \frac{I(n\mathbf{k},n'\mathbf{k})}{\varepsilon_{n\mathbf{k}} - \varepsilon_{n'\mathbf{k}}}. \tag{5.7.11b}$$

The (approximately) diagonal form of (5.7.9) implies that the thermal expectation values are

$$\langle \widetilde{c}^{+}_{n\mathbf{k}\sigma} \widetilde{c}_{n'\mathbf{k}'\sigma'}\rangle = \delta_{nn'}\delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}\, f_{n\mathbf{k}\sigma}, \tag{5.7.12a}$$

where

$$f_{n\mathbf{k}\sigma} = \frac{1}{e^{\beta(\widetilde{\varepsilon}_{n\mathbf{k}\sigma} - \mu_F)} + 1} \tag{5.7.12b}$$

is the *Fermi–Dirac distribution function* and μ_F is the chemical potential, equal to the Fermi energy $\widetilde{\varepsilon}_F$ in the temperature regime in which we shall be interested. The moment density is determined by (5.7.4), and introducing the new Fermi operators and using (5.7.12), we obtain

$$\begin{aligned}
\langle \mu_z(\mathbf{r})\rangle_{\text{c.el.}} &= \mu_B \sum_{nn'}\sum_{\mathbf{k}\mathbf{k}'} \psi^{*}_{n'\mathbf{k}'}(\mathbf{r})\psi_{n\mathbf{k}}(\mathbf{r})\big(\langle c^{+}_{n'\mathbf{k}'\uparrow} c_{n\mathbf{k}\uparrow}\rangle - \langle c^{+}_{n'\mathbf{k}'\downarrow} c_{n\mathbf{k}\downarrow}\rangle\big) \\
&= \mu_B \sum_{nn'}\sum_{\mathbf{k}} \psi^{*}_{n'\mathbf{k}}(\mathbf{r})\psi_{n\mathbf{k}}(\mathbf{r})\big[\{\delta_{nn'} + U^{*}_{\mathbf{k}}(n',n)\}(f_{n\mathbf{k}\uparrow} - f_{n\mathbf{k}\downarrow}) \\
&\qquad\qquad + U_{\mathbf{k}}(n,n')(f_{n'\mathbf{k}\uparrow} - f_{n'\mathbf{k}\downarrow})\big].
\end{aligned} \tag{5.7.13}$$

The uniform, averaged part of this moment density can be obtained by an integration of eqn (5.7.13) over space, and remembering that the wavefunctions are orthogonal and normalized, we find the magnetic moment of the conduction electrons per ion to be

$$\langle \mu_z\rangle_{\text{c.el.}} = \mu_B \frac{1}{N}\sum_{n\mathbf{k}}\big(f_{n\mathbf{k}\uparrow} - f_{n\mathbf{k}\downarrow}\big). \tag{5.7.14}$$

We note that, in addition to this uniform polarization of the conduction electrons, there is a spatially non-uniform component of the polarization density with the periodicity of the lattice. This non-uniform component reflects the variation in the electronic density, including the perturbative changes due to the *interband* contributions proportional to $U_{\mathbf{k}}(n,n')$. Furthermore, when the spin–orbit coupling of the conduction electrons is of importance, the interband coupling may induce a positional dependence in the direction of the spin polarization.

In order to obtain order-of-magnitude estimates of the exchange effects, we introduce a reasonable but somewhat crude approximation for the exchange integral, which is due to Overhauser (1963) and has been discussed in detail by Freeman (1972). First we assume that the Coulomb interaction in eqn (5.7.5) is strongly shielded, so that it can be replaced by a δ-function. Next, using plane waves for the Bloch functions, we obtain

$$(g-1)I(n\mathbf{k}', n\mathbf{k}) \approx j(\mathbf{q}=\mathbf{k}'-\mathbf{k}) \propto \int d\mathbf{r}|\phi_{4f}(\mathbf{r})|^2 e^{-i\mathbf{q}\cdot\mathbf{r}}, \qquad (5.7.15)$$

which is the form factor of the $4f$-electron density, approximately the same as the local moment density (4.1.15). In this simplified model, where the conduction electrons are assumed to be free-electron-like, the interband exchange integrals, in which $n' \neq n$, are obtained by adding reciprocal-lattice vectors $\boldsymbol{\tau}$ to $\mathbf{q}$ in eqn (5.7.15). In this model, we obtain a rigid band-splitting, independent of $\mathbf{k}$, between the spin-down and spin-up bands, of magnitude

$$\Delta = \widetilde{\varepsilon}_{n\mathbf{k}\downarrow} - \widetilde{\varepsilon}_{n\mathbf{k}\uparrow} = 2\langle J_z\rangle j(\mathbf{0}). \qquad (5.7.16)$$

Since $j(\mathbf{0})$ has the same sign as $(g-1)$, it is positive in the heavy rare earth metals. If $\mathcal{N}(\varepsilon)$ is the density of electronic states per ion and per spin state in the paramagnetic phase, the shifts of the spin-up and spin-down bands lead to an excess number of spin-up electrons proportional to

$$\overline{\mathcal{N}}(\widetilde{\varepsilon}_F) = \frac{1}{\Delta}\int_{\widetilde{\varepsilon}_F-\frac{\Delta}{2}}^{\widetilde{\varepsilon}_F+\frac{\Delta}{2}} \mathcal{N}(\varepsilon)d\varepsilon, \qquad (5.7.17)$$

when the small modification of the density of states due to the interband coupling is neglected, so that $\widetilde{\varepsilon}_F$ is close to the Fermi energy ε_F of the non-magnetic system. In combination with eqn (5.7.14), this result predicts a (positive) augmentation of the ferromagnetic moment of the $4f$ electrons, due to the conduction electrons, of magnitude

$$\langle\mu_z\rangle_{\text{c.el.}} = \mu_B\overline{\mathcal{N}}(\widetilde{\varepsilon}_F)\Delta, \qquad (5.7.18)$$

when $k_BT \ll \widetilde{\varepsilon}_F$. The total moment per ion may then be expressed in terms of an effective g-factor:

$$\langle\mu_z\rangle = g\mu_B\langle J_z\rangle + \langle\mu_z\rangle_{\text{c.el.}} = (g+\Delta g)\mu_B\langle J_z\rangle, \qquad (5.7.19a)$$

where

$$\Delta g = 2j(\mathbf{0})\overline{\mathcal{N}}(\widetilde{\varepsilon}_F). \qquad (5.7.19b)$$

In the metals, the effective exchange integral $j(\mathbf{0})$ is $\sim (g-1)\times 0.1\,\text{eV}$, leading to an exchange splitting Δ which, in Gd for example, is nearly 1 eV. This relatively large splitting has the consequence that $\overline{\mathcal{N}}(\widetilde{\varepsilon}_F)$ may differ somewhat from the value $\mathcal{N}(\varepsilon_F)$ in the paramagnetic phase. In the hcp metals, the band structure calculations discussed in Section 1.3 reveal that ε_F is near a peak in the density of states due to the d electrons, and that $\mathcal{N}(\varepsilon_F) \simeq 1\,\mathrm{eV}^{-1}$ per spin state per ion, corresponding to an electronic moment of the order of one-tenth of the local moment. In the example of Gd, for which $g = 2$, $\Delta g = 0.18$. The same value of $\Delta g/(g-1)$ accounts fairly well for the conduction-electron contribution to the moments of the other heavy rare earths in Table 1.6, bearing in mind the uncertainties in the experimental results, and the possible effects of the crystal fields in quenching the local moments.

The spin waves in the ferromagnetic phase are decisively influenced by the *sf*-exchange interaction. In order to consider such effects, we introduce the Bose operators acting on the angular-momentum states, as in eqns (5.2.6–8), and find, to first order in $1/J$,

$$\begin{aligned}\mathcal{H}_{sf} \simeq \mathcal{H}_{sf}(\mathrm{MF}) - \frac{1}{N}\sum_{\mathbf{kq}\boldsymbol{\tau}}\sum_{i} j(\mathbf{q}+\boldsymbol{\tau})\, e^{-i\mathbf{q}\cdot\mathbf{R}_i}\Big[&-\delta_{\mathbf{q}\mathbf{0}}((\langle c^+_{\mathbf{k}+\boldsymbol{\tau}\uparrow}c_{\mathbf{k}\uparrow}\rangle \\ &- \langle c^+_{\mathbf{k}+\boldsymbol{\tau}\downarrow}c_{\mathbf{k}\downarrow}\rangle))a_i^+a_i + \sqrt{2J}c^+_{\mathbf{k}+\mathbf{q}+\boldsymbol{\tau}\uparrow}c_{\mathbf{k}\downarrow}\,a_i^+ + \sqrt{2J}c^+_{\mathbf{k}+\mathbf{q}+\boldsymbol{\tau}\downarrow}c_{\mathbf{k}\uparrow}\,a_i\Big],\end{aligned}$$

using the simplified exchange of eqn (5.7.15), and neglecting effects of third or higher order in $j(\mathbf{q})$ due to $(c^+_{\mathbf{k}'\sigma}c_{\mathbf{k}\sigma} - \langle c^+_{\mathbf{k}'\sigma}c_{\mathbf{k}\sigma}\rangle)a_i^+a_i$. $\mathbf{q}$ is assumed to lie in the primitive Brillouin zone, but no such restriction is placed on $\mathbf{k}$. We note that $c^+_{\mathbf{k}}$ and $c^+_{\mathbf{k}+\boldsymbol{\tau}}$, where $\boldsymbol{\tau}$ is a reciprocal lattice vector, create electrons in different bands in the free-electron model. Introducing the crystal-field Hamiltonian to first order in $1/J$ (eqn (5.2.14) with $\mathcal{J}(ij) = 0$), and the Fourier transforms of the Bose operators (5.2.16), we find that the total magnetic Hamiltonian becomes

$$\begin{aligned}\mathcal{H} = \widetilde{\mathcal{H}}_s &+ \sum_{\mathbf{q}}\big[\{A + J\widetilde{\mathcal{J}}(\mathbf{0},0)\}a^+_{\mathbf{q}}a_{\mathbf{q}} + B\tfrac{1}{2}(a_{\mathbf{q}}a_{-\mathbf{q}} + a^+_{\mathbf{q}}a^+_{-\mathbf{q}})\big] \\ &- \sqrt{2J/N}\sum_{\mathbf{kq}\boldsymbol{\tau}} j(\mathbf{q}+\boldsymbol{\tau})\big(c^+_{\mathbf{k}+\mathbf{q}+\boldsymbol{\tau}\uparrow}c_{\mathbf{k}\downarrow}\,a^+_{-\mathbf{q}} + c^+_{\mathbf{k}+\mathbf{q}+\boldsymbol{\tau}\downarrow}c_{\mathbf{k}\uparrow}\,a_{\mathbf{q}}\big),\end{aligned} \tag{5.7.20}$$

where

$$\widetilde{\mathcal{J}}(\mathbf{0},0) = 2j^2(\mathbf{0})\overline{\mathcal{N}}(\widetilde{\varepsilon}_F) + \frac{2}{N}\sum_{\mathbf{k},\boldsymbol{\tau}\neq\mathbf{0}}|j(\boldsymbol{\tau})|^2\frac{f_{\mathbf{k}\downarrow} - f_{\mathbf{k}+\boldsymbol{\tau}\uparrow}}{\varepsilon_{\mathbf{k}+\boldsymbol{\tau}} - \varepsilon_{\mathbf{k}}}, \tag{5.7.21}$$

including the ‘interband’ contributions as in (5.7.9). The spin-wave energies may be obtained from the poles in the Green function $\langle\langle a_{\mathbf{q}}\,;\,a^+_{\mathbf{q}}\rangle\rangle$. The equation of motion (3.3.14) for this Green function is determined from $\mathcal{H}$ to be

$$\begin{aligned}\big\{\hbar\omega - A - J\widetilde{\mathcal{J}}(\mathbf{0},0)\big\}\langle\langle a_{\mathbf{q}}\,;a^+_{\mathbf{q}}\rangle\rangle - B\langle\langle a^+_{-\mathbf{q}}\,;a^+_{\mathbf{q}}\rangle\rangle \\ + \sqrt{2J/N}\sum_{\mathbf{k}\boldsymbol{\tau}} j(-\mathbf{q}-\boldsymbol{\tau})\langle\langle c^+_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}c_{\mathbf{k}\downarrow}\,;a^+_{\mathbf{q}}\rangle\rangle = 1.\end{aligned}\tag{5.7.22}$$

The equation of motion of the new Green function $\langle\langle c^+_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}c_{\mathbf{k}\downarrow}\,;a^+_{\mathbf{q}}\rangle\rangle$ involves the following commutator:

$$\begin{aligned}[c^+_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}c_{\mathbf{k}\downarrow}\,,\mathcal{H}\,] &= \big(\varepsilon_{\mathbf{k}\downarrow} - \varepsilon_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}\big)c^+_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}c_{\mathbf{k}\downarrow} \\ &\quad + \sqrt{2J/N}\sum_{\mathbf{q}'} j(\mathbf{q}')\big(c^+_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}+\mathbf{q}'\downarrow}c_{\mathbf{k}\downarrow} - c^+_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}c_{\mathbf{k}-\mathbf{q}'\uparrow}\big)\,a_{\mathbf{q}'} \\ &\simeq \big(\varepsilon_{\mathbf{k}\downarrow} - \varepsilon_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}\big)c^+_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}c_{\mathbf{k}\downarrow} + \sqrt{2J/N}\,j(\mathbf{q}+\boldsymbol{\tau})\big(f_{\mathbf{k}\downarrow} - f_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}\big)\,a_{\mathbf{q}}\end{aligned}\tag{5.7.23}$$

obtained by applying the anticommutator relations (5.7.3) and, in the second equation, an RPA decoupling of the operator products. It is not necessary here to differentiate between the new and the old Fermi operators, as the differences introduce corrections only in the third order of $|j(\mathbf{q})|$. Introducing this RPA result in the equation of motion for the Green function $\langle\langle c^+_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}c_{\mathbf{k}\downarrow}\,;a^+_{\mathbf{q}}\rangle\rangle$, we obtain

$$\begin{aligned}\big(\hbar\omega - \varepsilon_{\mathbf{k}\downarrow} + \varepsilon_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}\big)\langle\langle c^+_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}c_{\mathbf{k}\downarrow}\,;a^+_{\mathbf{q}}\rangle\rangle \\ - \sqrt{2J/N}\,j(\mathbf{q}+\boldsymbol{\tau})\big(f_{\mathbf{k}\downarrow} - f_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}\big)\langle\langle a_{\mathbf{q}}\,;a^+_{\mathbf{q}}\rangle\rangle = 0,\end{aligned}\tag{5.7.24}$$

which, in combination with (5.7.22), leads to

$$\big\{\hbar\omega - A - J\widetilde{\mathcal{J}}(\mathbf{0},0) + J\widetilde{\mathcal{J}}(\mathbf{q},\omega)\big\}\langle\langle a_{\mathbf{q}}\,;a^+_{\mathbf{q}}\rangle\rangle - B\langle\langle a^+_{-\mathbf{q}}\,;a^+_{\mathbf{q}}\rangle\rangle = 1,\tag{5.7.25}$$

where

$$\widetilde{\mathcal{J}}(\mathbf{q},\omega) = \lim_{\varepsilon\to 0^+}\frac{2}{N}\sum_{\boldsymbol{\tau}}|j(\mathbf{q}+\boldsymbol{\tau})|^2\sum_{\mathbf{k}}\frac{f_{\mathbf{k}\downarrow} - f_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}}{\hbar\omega + i\hbar\varepsilon - \varepsilon_{\mathbf{k}\downarrow} + \varepsilon_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow}}.\tag{5.7.26a}$$

This result may be expressed in terms of the susceptibility of the conduction electrons. Introducing the spin susceptibility per ion, which is the usual magnetic susceptibility times $(2\mu_B)^{-2}V/N$, so that

$$\begin{aligned}\chi^{+-}_{\text{c.el.}}(\mathbf{q},\omega) &= -\frac{1}{N}\int d\mathbf{r}_1 d\mathbf{r}_2\langle\langle s^+(\mathbf{r}_1)\,;s^-(\mathbf{r}_2)\rangle\rangle\, e^{-i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \\ &= -\frac{1}{N}\sum_{\mathbf{k}'\mathbf{k}''}\langle\langle c^+_{\mathbf{k}'-\mathbf{q}\uparrow}c_{\mathbf{k}'\downarrow}\,;c^+_{\mathbf{k}''+\mathbf{q}\downarrow}c_{k''\uparrow}\rangle\rangle \\ &= \lim_{\varepsilon\to 0^+}\frac{1}{N}\sum_{\mathbf{k}}\frac{f_{\mathbf{k}\downarrow} - f_{\mathbf{k}-\mathbf{q}\uparrow}}{\hbar\omega + i\hbar\varepsilon - \varepsilon_{\mathbf{k}\downarrow} + \varepsilon_{\mathbf{k}-\mathbf{q}\uparrow}},\end{aligned}\tag{5.7.26b}$$

and neglecting the higher-order corrections to the spin-susceptibility, due to the coupling to the local moments, we can write the above result

$$\widetilde{\mathcal{J}}(\mathbf{q},\omega) = 2\sum_{\boldsymbol{\tau}} |j(\mathbf{q}+\boldsymbol{\tau})|^2 \chi^{+-}_{\text{c.el.}}(\mathbf{q}+\boldsymbol{\tau},\omega), \tag{5.7.26c}$$

where by the relation (3.2.15), $\chi^{+-}_{\text{c.el.}}(\mathbf{q},\omega) = [\chi^{-+}_{\text{c.el.}}(-\mathbf{q},-\omega)]^*$. In general, when the Coulomb interaction cannot be approximated by a δ-function, this factorization is not valid, and the indirect exchange is instead given by

$$\widetilde{\mathcal{J}}(\mathbf{q},\omega) = \lim_{\varepsilon\to 0^+} \frac{2}{N}\sum_{nn'}\sum_{\mathbf{k}} (g-1)^2 |I(n'\mathbf{k}-\mathbf{q},n\mathbf{k})|^2 \frac{f_{n\mathbf{k}\downarrow} - f_{n'\mathbf{k}-\mathbf{q}\uparrow}}{\hbar\omega + i\hbar\varepsilon - \varepsilon_{n\mathbf{k}\downarrow} + \varepsilon_{n'\mathbf{k}-\mathbf{q}\uparrow}}, \tag{5.7.27}$$

where $\mathbf{k}$ is now confined to the primitive Brillouin zone.

In the frequency regime of the spin waves, where $|\hbar\omega|$ is much smaller than the Fermi energy or the exchange splitting Δ, the frequency dependence of $\widetilde{\mathcal{J}}(\mathbf{q},\omega)$ can, to a good approximation, be neglected. The spins of the conduction electrons respond essentially instantaneously to any changes in the state of the local angular momenta, compared with the time-scale of these changes. For a Bravais-lattice, $\widetilde{\mathcal{J}}(\mathbf{q},\omega) \simeq \widetilde{\mathcal{J}}(\mathbf{q},0) = \widetilde{\mathcal{J}}(-\mathbf{q},0)$. A comparison of eqn (5.7.25) with the $1/J$ spin-wave result (5.2.18) shows that $\widetilde{\mathcal{J}}(\mathbf{0},0) - \widetilde{\mathcal{J}}(\mathbf{q},0)$ replaces the contribution of the Heisenberg interaction considered in eqn (5.2.1). In this equation, $\mathcal{J}(ii) \equiv 0$ by definition and, since this is not the case for $\widetilde{\mathcal{J}}(ii) = (1/N)\sum_{\mathbf{q}}\widetilde{\mathcal{J}}(\mathbf{q},0)$, $\widetilde{\mathcal{J}}(\mathbf{q},0)$ cannot be associated directly with $\mathcal{J}(\mathbf{q})$. The instantaneous or frequency-independent part of the coupling of $\mathbf{J}_i$ with itself leads to a contribution $\frac{1}{2}N\widetilde{\mathcal{J}}(ii)\langle\mathbf{J}_i\cdot\mathbf{J}_i\rangle$ to the total energy, where $\langle\mathbf{J}_i\cdot\mathbf{J}_i\rangle = J(J+1)$, independently of the magnetic ordering or the temperature. This assertion may be verified (to first order in $1/J$) by a direct calculation of $\langle\mathcal{H}\rangle$ from (5.7.20). For this purpose $\langle c^+_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\uparrow} c_{\mathbf{k}\downarrow} a^+_{\mathbf{q}}\rangle$, for instance, is determined from eqn (5.7.24), but a *self-energy* correction of a factor 1/2 must be included in its contribution to $\langle\mathcal{H}\rangle$. Taking this condition into account, we may finally write

$$\mathcal{J}(\mathbf{q}) = \widetilde{\mathcal{J}}(\mathbf{q},0) - \frac{1}{N}\sum_{\mathbf{q}'}\widetilde{\mathcal{J}}(\mathbf{q}',0). \tag{5.7.28}$$

The exchange interaction between the $4f$ electrons and the conduction electrons thus leads to an effective Heisenberg interaction between the local angular momenta, as given in (5.2.1). This is the RKKY interaction discussed earlier in Section 1.4.

The above calculation has been performed for a Bravais lattice, but the result (5.7.26) is readily generalized to a crystal with a basis of p ions, as the conduction electrons, in the approximation adopted, are not affected by the presence of the basis. If the couplings between the different sublattices are introduced in an equivalent manner to (5.1.1), then

$$\widetilde{\mathcal{J}}_{ss'}(\mathbf{q},\omega) = \frac{2}{p}\sum_{\boldsymbol{\tau}} |j(\mathbf{q}+\boldsymbol{\tau})|^2 \chi^{+-}_{\text{c.el.}}(\mathbf{q}+\boldsymbol{\tau},\omega)\exp\big(i\boldsymbol{\rho}_{ss'}\cdot\boldsymbol{\tau}\big) \qquad (5.7.29)$$

replaces (5.7.26c), where $\boldsymbol{\rho}_{ss'}$ is the vector connecting the two sublattices s and s'.

The interaction between the localized moments is effectuated via virtual electron-hole pair-excitations of the conduction electrons. The transmission of any time-dependent event may be disturbed in two ways; either by the finite propagation-time of the pairs, or by a decay of the pair states into unbound electron and hole excitations, the so-called *Stoner* excitations. The second effect produces by far the most important correction to the instantaneous interaction, but we shall begin with a discussion of the frequency-dependence of the real part of $\widetilde{\mathcal{J}}(\mathbf{q},\omega)$, due to the finite transmission time. Returning to the simple model leading to (5.7.26), we find that the exchange coupling is proportional to the susceptibility function $\chi^{+-}_{\text{c.el.}}(\mathbf{q},\omega)$, which for unpolarized free electrons is the same as the *Lindhard function* (Lindhard 1954). If corrections of the order k_BT/ε_F are neglected, the real part at zero wave-vector is

$$\begin{aligned}\text{Re}\big[\chi^{+-}_{\text{c.el.}}(\mathbf{0},\omega)\big] &= \frac{1}{N}\sum_{\mathbf{k}}\frac{f_{\mathbf{k}\downarrow}-f_{\mathbf{k}\uparrow}}{\hbar\omega-\varepsilon_{\mathbf{k}\downarrow}+\varepsilon_{\mathbf{k}\uparrow}} \\ &= \frac{1}{N}\sum_{\mathbf{k}}\frac{f_{\mathbf{k}\uparrow}-f_{\mathbf{k}\downarrow}}{\Delta-\hbar\omega} = \overline{\mathcal{N}}(\widetilde{\epsilon}_F)\Big(1+\frac{\hbar\omega}{\Delta}\Big).\end{aligned} \qquad (5.7.30)$$

From this result, we find immediately that the intra-band contribution at zero frequency to $\widetilde{\mathcal{J}}(\mathbf{q}\rightarrow\mathbf{0},0)$ in eqn (5.7.26a) is $2j^2(\mathbf{0})\overline{\mathcal{N}}(\widetilde{\epsilon}_F)$, which is the same as in (5.7.21). On the other hand, the interband contributions differ in the two expressions, as the denominator in (5.7.26a) involves the exchange splitting Δ, whereas that in (5.7.21) does not. However, this difference can be neglected, as it is of the order $(\Delta/\varepsilon_F)^2$ times the intra-band contribution, which is beyond the order considered in these calculations. In fact, since the starting Hamiltonian (5.7.6) is invariant with respect to the choice of z-axis for the electronic spins and the angular momenta, the spin-wave frequency must vanish when $\mathbf{q}\rightarrow\mathbf{0}$ and $A = B = 0$, according to the *Goldstone theorem*, which will be discussed in the next chapter. Therefore $\widetilde{\mathcal{J}}(\mathbf{q}\rightarrow\mathbf{0},0) = \widetilde{\mathcal{J}}(\mathbf{0},0)$, and we simply assume that eqn (5.7.26a), with $(\mathbf{q},\omega)=(\mathbf{0},0)$, replaces eqn (5.7.21). In the presence of an external field, Δ in eqn (5.7.16) is increased by an amount $2\mu_B H$, which leads to the extra contribution $\Delta g\mu_B H$ to $\widetilde{\mathcal{J}}(\mathbf{0},0)$ in (5.7.21), as the change with field of the interband terms may be neglected. To leading order, $\widetilde{\mathcal{J}}(\mathbf{q}\to\mathbf{0},0)$ is not affected by the applied field, so to this order the extra polarization of the conduction electrons, due to an external field, may simply be accounted for by replacing $g\mu_B H$ by $(g+\Delta g)\mu_B H$, both in the Zeeman energy (5.7.19a) and in the spin-wave energy parameters (in A). Writing the susceptibility in eqn (5.7.26b) as the sum of two terms, and replacing $\mathbf{k}-\mathbf{q}$ by $\mathbf{k}$ in the term involving $f_{\mathbf{k}-\mathbf{q}\uparrow}$, we obtain

$$\begin{aligned}\mathrm{Re}\big[\chi^{+-}_{\text{c.el.}}(\mathbf{q},\omega)\big] = \\ &\frac{V}{(2\pi)^3}\frac{2\pi}{N}\int_0^{k_{F\downarrow}} k^2dk\int_{-1}^{1} d\mu\big[\hbar\omega-\Delta+\frac{(\hbar q)^2}{2m}-\frac{\hbar^2kq}{m}\mu\big]^{-1} \\ &-\frac{V}{(2\pi)^3}\frac{2\pi}{N}\int_0^{k_{F\uparrow}} k^2dk\int_{-1}^{1} d\mu\big[\hbar\omega-\Delta-\frac{(\hbar q)^2}{2m}-\frac{\hbar^2kq}{m}\mu\big]^{-1},\end{aligned}$$

or

$$\mathrm{Re}\big[\chi^{+-}_{\text{c.el.}}(\mathbf{q},\omega)\big] = \frac{V}{N}\frac{m}{(2\pi\hbar)^2}\Big\{k_{F\downarrow}(1-\eta)\mathcal{F}\Big(\frac{q}{2k_{F\downarrow}}(1-\eta)\Big)+k_{F\uparrow}(1+\eta)\mathcal{F}\Big(\frac{q}{2k_{F\uparrow}}(1+\eta)\Big)\Big\} \tag{5.7.31a}$$

where we have introduced the function

$$\mathcal{F}(x)=\frac{1}{2}+\frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right| \tag{5.7.31b}$$

and the parameter

$$\eta=\frac{\Delta-\hbar\omega}{\varepsilon_F}\left(\frac{k_F}{q}\right)^2. \tag{5.7.31c}$$

The Fermi energy is $\varepsilon_F=(\hbar k_F)^2/2m$, and the wave-vectors of the spin-up and the spin-down electrons at the Fermi surface are

$$k_{F\uparrow}=k_F\big(1+\frac{\Delta}{2\varepsilon_F}\big)^{\frac{1}{2}} \quad ; \quad k_{F\downarrow}=k_F\big(1-\frac{\Delta}{2\varepsilon_F}\big)^{\frac{1}{2}}. \tag{5.7.31d}$$

$\eta\to\infty$ in the limit $q\to 0$ and, using $\mathcal{F}(x)=1/3x^2$ when $|x|\to\infty$, we may re-derive the result (5.7.30). At non-zero q, a numerical analysis shows that, to a good approximation,

$$\mathrm{Re}\big[\chi^{+-}_{\text{c.el.}}(\mathbf{q},\omega)\big]=\overline{\mathcal{N}}(\widetilde{\epsilon}_F)\Big\{\mathcal{F}\big(\frac{q}{2k_F}\big)+\xi_q\frac{\hbar\omega}{\Delta}\Big\}, \tag{5.7.32}$$

even when Δ/ε_F is as large as 0.5. The parameter ξ_q is equal to 1 at $q = 0$, and peaks at $q = q_0 = k_{F\uparrow} - k_{F\downarrow}$, after which it rapidly decreases ($\xi_q \simeq 0.25$ at $q = 2q_0$). For $\Delta/\varepsilon_F = 0.1$, the maximum value is about 4 and it decreases for increasing values of Δ, falling to about 3 at $\Delta/\varepsilon_F = 0.4$. Usually q_0 is much smaller than the length of any reciprocal-lattice vector, which means that the frequency dependence of the 'interband' term in the real part of $\widetilde{\mathcal{J}}(\mathbf{q},\omega)$ can be neglected. The intra-band contribution is $2|j(\mathbf{q})|^2\overline{\mathcal{N}}(\widetilde{\epsilon}_F)\xi_q\hbar\omega/\Delta$, and using

$$\big\{\hbar\omega + A + J\widetilde{\mathcal{J}}(\mathbf{0},0) - J\widetilde{\mathcal{J}}^*(-\mathbf{q},-\omega)\big\}\langle\langle a^+_{-\mathbf{q}}\,;\,a^+_{\mathbf{q}}\rangle\rangle + B\langle\langle a_{\mathbf{q}}\,;\,a^+_{\mathbf{q}}\rangle\rangle = 0, \tag{5.7.33}$$

which follows by symmetry from eqn (5.7.25), we may determine the spin-wave energies from the real part of $\widetilde{\mathcal{J}}(\mathbf{q},\omega)$ to be

$$\hbar\omega = E'_{\mathbf{q}} = E_{\mathbf{q}}\big[1 + \xi_q\overline{\mathcal{N}}(\widetilde{\epsilon}_F)|j(\mathbf{q})|^2/j(\mathbf{0})\big]^{-1}, \tag{5.7.34a}$$

to first order in $1/J$, with $E_{\mathbf{q}}$ given by (5.2.22). The extra factor, which originates from the frequency dependence of $\chi^{+-}_{\mathrm{c.el.}}(\mathbf{q},\omega)$, differs from 1 by only a few per cent, and its $\mathbf{q}$-dependent contribution could scarcely be distinguished from that of $\mathcal{J}(\mathbf{q})$. However, the presence of this factor at $\mathbf{q} = \mathbf{0}$ means that the energy of the uniform spin-wave mode is no longer determined exclusively by the magnetic anisotropy of the bulk, according to (5.4.12) and (5.4.19), when the magnetoelastic effects are included, but instead the energy gap is

$$E'_{\mathbf{0}} = \frac{1}{N}\left(\frac{\partial^2 F}{\partial\theta^2}\frac{\partial^2 F}{\partial\phi^2}\bigg|_{\bar{\epsilon}}\right)^{\frac{1}{2}}\frac{1}{\langle J_z\rangle(1+\frac{1}{2}\Delta g)}. \tag{5.7.34b}$$

Although this modification is small, it demonstrates that the frequency dependence of $\chi^{+-}_{\mathrm{c.el.}}(\mathbf{q},\omega)$ may cause small deviations between the static anisotropy parameters and those derived from the energy gap, as possibly detected in Tb in the form of a non-zero value of $\delta_6(-)$, defined by eqn (5.4.23a).

The dominant term in the real part of $\chi^{+-}_{\mathrm{c.el.}}(\mathbf{q},\omega)$ is the frequency-independent contribution proportional to $\mathcal{F}(q/2k_F)$. Including only this contribution, and making the rather drastic simplifying assumption that $|j(\mathbf{q}+\boldsymbol{\tau})|$ in eqn (5.7.26c) is a constant $|j_0|$ at all wave-vectors, we may derive the exchange coupling in real space, which then depends only on the distance R between the different ions:

$$\mathcal{J}(R) = 2|j_0|^2\frac{V}{N(2\pi)^3}\int\overline{\mathcal{N}}(\widetilde{\epsilon}_F)\mathcal{F}\big(\frac{q}{2k_F}\big)e^{i\mathbf{q}\cdot\mathbf{R}}d\mathbf{q}.$$

The sum over $\boldsymbol{\tau}$ in (5.7.26c) corresponds to letting q vary between 0 and ∞, and the result is

$$\mathcal{J}(R) = 12\pi\nu|j_0|^2\overline{\mathcal{N}}(\widetilde{\epsilon}_F)\,\frac{\sin(2k_FR) - 2k_FR\cos(2k_FR)}{(2k_FR)^4}\,, \qquad (5.7.35)$$

where ν is the number of conduction electrons per ion; $\nu = Vk_F^3/3\pi^2N$. Although this result is not directly applicable to realistic systems, it demonstrates explicitly that the indirect coupling mediated by the conduction electrons is long range, $\mathcal{J}(R) \propto R^{-3}$ for large R, and that it oscillates. The period of the oscillation is here $2\pi/2k_F$ whereas, in a real system, such oscillations may occur as a result of large parallel areas of Fermi surface, the separation of which determines an effective value of $2k_F$. It is interesting that $\mathcal{J}(R)$, derived from the excitation spectrum in Pr and shown in Fig. 1.18 on page 49, is reasonably well described by the above function, especially when $\mathbf{R}$ is in the basal plane, provided that an effective value of $2k_F$ of about $1.1\,\text{Å}^{-1}$ is used.

The magnetic scattering of the electron-hole pairs leads to a damping of the spin waves, which is determined by the imaginary part of the susceptibility (5.7.26b). The complementary result to eqn (5.7.31a) is then

$$\begin{aligned}&\mathrm{Im}\big[\chi^{+-}_{\text{c.el.}}(\mathbf{q},\omega)\big] = \\ &-\frac{V}{(2\pi)^3}\frac{2\pi}{N}\int_0^\infty k^2dk\int_{-1}^1 d\mu\,\pi\delta\big(\hbar\omega - \Delta + \frac{(\hbar q)^2}{2m} - \frac{\hbar^2kq}{m}\mu\big)\,f_{\mathbf{k}\downarrow} \\ &+\frac{V}{(2\pi)^3}\frac{2\pi}{N}\int_0^\infty k^2dk\int_{-1}^1 d\mu\,\pi\delta\big(\hbar\omega - \Delta - \frac{(\hbar q)^2}{2m} - \frac{\hbar^2kq}{m}\mu\big)\,f_{\mathbf{k}\uparrow}.\end{aligned}$$

Because $-1 < \mu < 1$, the δ-function argument in the first term can only be zero if $\varepsilon_q \equiv (\hbar q)^2/(2m)$ lies between the two roots $\varepsilon_\pm = 2\varepsilon_k + \Delta - \hbar\omega \pm 2\big[\varepsilon_k(\varepsilon_k + \Delta - \hbar\omega)\big]^{1/2}$. For the second term, the same condition applies, except that the signs of Δ and $\hbar\omega$ are reversed, leading to the extra requirement that $\varepsilon_k > \varepsilon_K = \Delta - \hbar\omega$. If these conditions are satisfied,

$$\begin{aligned}&\mathrm{Im}\big[\chi^{+-}_{\text{c.el.}}(\mathbf{q},\omega)\big] = \\ &-\frac{V}{N(2\pi)^2}\int_0^\infty \frac{\pi m}{\hbar^2q}kf(\varepsilon_k + \tfrac{\Delta}{2})dk + \frac{V}{N(2\pi)^2}\int_K^\infty \frac{\pi m}{\hbar^2q}kf(\varepsilon_k - \tfrac{\Delta}{2})dk,\end{aligned}$$

where $f(\varepsilon) = 1/\big[\exp(\varepsilon - \varepsilon_F) + 1\big]$. By a suitable change of variables, the two integrals acquire the same limits and the same condition on ε_q, and they may therefore be combined in a single integral:

$$\mathrm{Im}\big[\chi^{+-}_{\text{c.el.}}(\mathbf{q},\omega)\big] = \frac{V}{N(2\pi)^2}\frac{\pi m^2}{\hbar^4q}\int_{\frac{\Delta-\hbar\omega}{2}}^\infty \big\{-f(\varepsilon + \tfrac{\hbar\omega}{2}) + f(\varepsilon - \tfrac{\hbar\omega}{2})\big\}d\varepsilon.$$

The integrand is only non-zero in a narrow interval of width $|\hbar\omega| \ll \Delta < \varepsilon_F$ around the Fermi surface, in which case the condition on ε_q can be written $k_{F\uparrow} - k_{F\downarrow} < q < k_{F\uparrow} + k_{F\downarrow}$ (if $\Delta = 0$ the lower boundary is replaced by $(\hbar\omega)^2/(4\varepsilon_F) < \varepsilon_q$). With this condition fulfilled,

$$\mathrm{Im}\big[\chi^{+-}_{\mathrm{c.el.}}(\mathbf{q},\omega)\big] = \frac{V}{N(2\pi)^2}\frac{\pi m^2}{\hbar^4 q}\hbar\omega,$$

independent of T (as long as $k_BT \ll \varepsilon_F$). Using

$$\mathcal{N}_\sigma(\varepsilon_F) = (V/N)(2\pi\hbar)^{-2}2mk_{F\sigma} \quad ; \quad (V/N)(2\pi)^{-2}\,\tfrac{2}{3}(k^3_{F\uparrow} + k^3_{F\downarrow}) = \nu,$$

where ν is the number of conduction electrons per ion ($\nu = 3$), we may write the result:

$$\mathrm{Im}\big[\chi^{+-}_{\mathrm{c.el.}}(\mathbf{q},\omega)\big] = \frac{\pi}{3\nu}\mathcal{N}_\uparrow(\varepsilon_F)\mathcal{N}_\downarrow(\varepsilon_F)\frac{k_F}{q}\hbar\omega; \qquad (5.7.36)$$
$$k_{F\uparrow} - k_{F\downarrow} < q < k_{F\uparrow} + k_{F\downarrow},$$

neglecting corrections of second order in Δ/ε_F. In the zero-frequency limit considered here, q has to exceed the threshold value $q_0 = k_{F\uparrow} - k_{F\downarrow}$ before the imaginary part of $\chi^{+-}_{\mathrm{c.el.}}(\mathbf{q},\omega)$ becomes non-zero. This threshold value corresponds to the smallest distance in q-space between an occupied spin-down state and an unoccupied spin-up state, or vice versa, of nearly the same energy ($\simeq \varepsilon_F$). At $q = q_0$, the function makes a discontinuous step from zero to a finite value. The above result, combined with eqn (5.7.26), leads to

$$\mathrm{Im}\big[\widetilde{\mathcal{J}}(\mathbf{q},\omega)\big] = \zeta(\mathbf{q})\hbar\omega, \qquad (5.7.37a)$$

with

$$\zeta(\mathbf{q}) = \frac{2\pi}{3\nu}\mathcal{N}_\uparrow(\varepsilon_F)\mathcal{N}_\downarrow(\varepsilon_F)\sum_{\boldsymbol{\tau}}|j(\mathbf{q}+\boldsymbol{\tau})|^2\frac{k_F}{|\mathbf{q}+\boldsymbol{\tau}|}, \qquad (5.7.37b)$$

where the sum is restricted to $k_{F\uparrow} - k_{F\downarrow} < |\mathbf{q}+\boldsymbol{\tau}| < k_{F\uparrow} + k_{F\downarrow}$. The imaginary part of $\widetilde{\mathcal{J}}(\mathbf{q},\omega)$ gives rise to a non-zero width in the spin-wave excitations. If the above result is inserted in eqns (5.7.25) and (5.7.33), the denominator of the Green functions may approximately be written $(\hbar\omega)^2 - (E'_{\mathbf{q}})^2 + 2i\Gamma_{\mathbf{q}}\hbar\omega$, where $\Gamma_{\mathbf{q}}$ is half the linewidth of the spin waves at the wave-vector $\mathbf{q}$, and is found to take the form

$$\Gamma_{\mathbf{q}} = J\big[A + J\{\mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q})\}\big]\,\zeta(\mathbf{q}) = JA_{\mathbf{q}}\,\zeta(\mathbf{q}). \qquad (5.7.38)$$

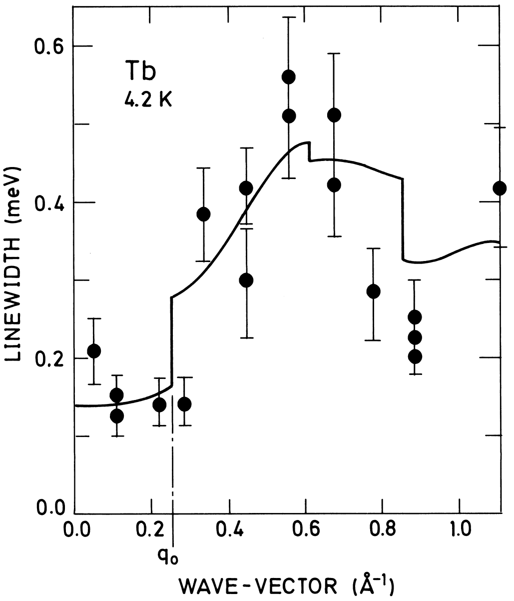

Fig. 5.13. The linewidths of magnons propagating in the c-direction of Tb at 4 K, compared with a theory based upon the nearly-free-electron model. The abrupt changes in the calculated lifetimes are due to the spin-splitting of the Fermi surface.

The lifetimes of the magnons propagating in the c-direction in Tb at 4 K, at which temperature the conduction electrons provide the dominant scattering process, were measured by Bjerrum Møller and Mackintosh (1979). As illustrated in Fig. 5.13, the linewidths are small, but non-zero, at small wave-vectors, rise abruptly at about a quarter of the way to the zone boundary, and fall again at large q. In order to interpret these results rigorously, it would be necessary to use eqn (5.7.27), with the correct band structure for Tb and realistic values for the exchange matrix elements $I(n'\mathbf{k}', n\mathbf{k})$. However, it is possible to obtain a semi-quantitative description by using the simple free-electron expression (5.7.37). As we shall see in the remainder of this section, this model, with an sf-interaction determined, for example, from the polarization of the conduction electrons (5.7.16–19), gives a surprisingly good account of the real scattering processes involving the interaction between the $4f$ and conduction electrons. Although the dominant d bands are far from parabolic in the rare earths, the nearly-free-electron Fermi surface for a trivalent hcp metal has a sheet with the form of a lens normal to the c-axis (Mackintosh *et al.* 1963), which mimics the Fermi-surface webbing described in Section 1.3, and reproduces a number of observed features. In the calculations of Jensen (1982a), compared with the experimental results in Fig. 5.13, the spin-splitting of this surface gives rise to the critical value q_0 at which the linewidths abruptly increase. The finite lifetimes below this cut-off are due to interband transitions between states on sections of the Fermi surface with opposite spin, which intersect in the primitive Brillouin zone after translation through a reciprocal-lattice vector. These effects will also occur in calculations based on a realistic band structure, whereas the behaviour at higher q is much more dependent on the details of the energy bands.

5.7.2 The mass-enhancement of the conduction electrons

The processes in which the spin waves are scattered by the electron-hole pair excitations of the conduction electrons, and which therefore limit their lifetime, also have consequences for the conduction electrons. The energies of the conduction electrons are changed, and hence also their effective mass at the Fermi surface m^*, as measured directly by cyclotron resonance or the de Haas–van Alphen effect, or as determined from the low-temperature heat capacity. In the zero-temperature limit, the electronic part of the specific heat is

$$C = \gamma T = \frac{m^*}{m}\gamma_0 T \qquad ; \quad \gamma_0 = \tfrac{1}{3}\pi^2 k_B^2 \{\mathcal{N}_\uparrow(\widetilde{\varepsilon}_F) + \mathcal{N}_\downarrow(\widetilde{\varepsilon}_F)\}N, \quad (5.7.39)$$

where $m^* = (m^*_\uparrow + m^*_\downarrow)/2$ in the spin-polarized case. The use of $\widetilde{\varepsilon}_F$ instead of ε_F is meant to indicate that all the effects of the MF Hamiltonian, including the interband couplings in (5.7.7), are assumed to be incorporated in γ_0 or m.

In order to calculate m^*, we shall utilize the Green functions of the conduction electrons. Because these particles are fermions, it is convenient to introduce an alternative type of Green function, in which an anticommutator bracket replaces the commutator bracket occurring in the definition (3.3.12), so that, for instance,

$$G_\uparrow(\mathbf{k}, t-t') \equiv \langle\langle c_{\mathbf{k}\uparrow}(t)\,;\, c^+_{\mathbf{k}\uparrow}(t')\rangle\rangle_+ = -\frac{i}{\hbar}\theta(t-t')\langle\{c_{\mathbf{k}\uparrow}(t)\,,\, c^+_{\mathbf{k}\uparrow}(t')\}\rangle. \quad (5.7.40)$$

The Fourier transform obeys an equation of motion equivalent to eqn (3.3.14*a*), except that the commutator on the *right*-hand side of this equation is replaced by the anticommutator, or

$$\hbar\omega G_\uparrow(\mathbf{k},\omega) - \langle\langle[\,c_{\mathbf{k}\uparrow}\,,\,\mathcal{H}\,]\,;\, c^+_{\mathbf{k}\uparrow}\rangle\rangle_+ = \langle\{c_{\mathbf{k}\uparrow}\,,\, c^+_{\mathbf{k}\uparrow}\}\rangle = 1. \quad (5.7.41)$$

If $\mathcal{H}$ is approximated by $\widetilde{\mathcal{H}}_s$, given by eqn (5.7.10), we obtain the non-interacting value of the Green function

$$G_\uparrow(\mathbf{k},\omega) \simeq G^o_\uparrow(\mathbf{k},\omega) = \frac{1}{\hbar\omega - \varepsilon_{\mathbf{k}\uparrow}} \quad (5.7.42)$$

(neglecting the minor difference between ε and $\widetilde{\varepsilon}$), showing that the poles of the Green function determine the energies of the conduction electrons. Considering the total Hamiltonian, in the approximation given by (5.7.20), we have instead

$$(\hbar\omega - \varepsilon_{\mathbf{k}\uparrow})G_{\uparrow}(\mathbf{k},\omega) + \sqrt{2J/N}\sum_{\mathbf{q}\boldsymbol{\tau}} j(\mathbf{q}+\boldsymbol{\tau})\langle\langle c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}a^{+}_{-\mathbf{q}}\,;\,c^{+}_{\mathbf{k}\uparrow}\rangle\rangle_{+} = 1. \tag{5.7.43}$$

The equation of motion of the new Green function is determined from

$$\begin{aligned}
&[\,c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}a^{+}_{-\mathbf{q}}\,,\,\mathcal{H}\,] \\
&= \big\{\varepsilon_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow} - A - J\widetilde{\mathcal{J}}(\mathbf{0},0)\big\}c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}a^{+}_{-\mathbf{q}} - B\,c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}a_{\mathbf{q}} \\
&\quad - \sqrt{2J/N}\sum_{\mathbf{k}'\boldsymbol{\tau}'} j(-\mathbf{q}-\boldsymbol{\tau}')\Big[c^{+}_{\mathbf{k}'-\mathbf{q}-\boldsymbol{\tau}'\downarrow}c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}c_{\mathbf{k}'\uparrow} \\
&\qquad\qquad + \delta_{\mathbf{k}-\boldsymbol{\tau},\mathbf{k}'-\boldsymbol{\tau}'}\,\langle a^{+}_{-\mathbf{q}}a_{-\mathbf{q}}\rangle c_{\mathbf{k}+\boldsymbol{\tau}'-\boldsymbol{\tau}\uparrow}\Big],
\end{aligned}$$

using an RPA decoupling procedure to obtain the last term. To proceed further, we have to calculate $\langle\langle c^{+}_{\mathbf{k}'-\mathbf{q}-\boldsymbol{\tau}'\downarrow}c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}c_{\mathbf{k}'\uparrow}\,;\,c^{+}_{\mathbf{k}\uparrow}\rangle\rangle_{+}$ and, within the RPA,

$$\begin{aligned}
&\langle\langle c^{+}_{\mathbf{k}'-\mathbf{q}-\boldsymbol{\tau}'\downarrow}c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}c_{\mathbf{k}'\uparrow}\,;\,c^{+}_{\mathbf{k}\uparrow}\rangle\rangle_{+} \\
&= \delta_{\mathbf{k}'-\boldsymbol{\tau}',\mathbf{k}-\boldsymbol{\tau}}\,f_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}\langle\langle c_{\mathbf{k}+\boldsymbol{\tau}'-\boldsymbol{\tau}\uparrow}\,;\,c_{\mathbf{k}\uparrow}\rangle\rangle_{+} \\
&\quad - \sqrt{2J/N}\,\frac{j(\mathbf{q}+\boldsymbol{\tau}')\{f_{\mathbf{k}'\uparrow} - f_{\mathbf{k}'-\mathbf{q}-\boldsymbol{\tau}'\downarrow}\}}{\hbar\omega - \varepsilon_{\mathbf{k}'\uparrow} - \varepsilon_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow} + \varepsilon_{\mathbf{k}'-\mathbf{q}-\boldsymbol{\tau}'\downarrow}}\langle\langle c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}a^{+}_{-\mathbf{q}}\,;\,c^{+}_{\mathbf{k}\uparrow}\rangle\rangle_{+}.
\end{aligned}$$

Writing $\hbar\omega_1 = \hbar\omega - \varepsilon_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}$, we obtain from these equations

$$\begin{aligned}
&\big\{\hbar\omega_1 + A + J\widetilde{\mathcal{J}}(\mathbf{0},0) - J\widetilde{\mathcal{J}}^{*}(\mathbf{q},-\omega_1)\big\}\langle\langle c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}a^{+}_{-\mathbf{q}}\,;\,c^{+}_{\mathbf{k}\uparrow}\rangle\rangle_{+} \\
&\qquad\qquad + B\langle\langle c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}a_{\mathbf{q}}\,;\,c^{+}_{\mathbf{k}\uparrow}\rangle\rangle_{+} \\
&= -\sqrt{2J/N}\sum_{\boldsymbol{\tau}'} j(-\mathbf{q}-\boldsymbol{\tau}')\big(f_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow} + \langle a^{+}_{-\mathbf{q}}a_{-\mathbf{q}}\rangle\big)\langle\langle c_{\mathbf{k}+\boldsymbol{\tau}'-\boldsymbol{\tau}\uparrow}\,;\,c^{+}_{\mathbf{k}\uparrow}\rangle\rangle_{+}.
\end{aligned} \tag{5.7.44}$$

In the sum, the terms with $\boldsymbol{\tau}' \neq \boldsymbol{\tau}$ only lead to higher-order corrections, of the same type as those arising from the difference between $c_{\mathbf{k}\uparrow}$ and $\widetilde{c}_{\mathbf{k}\uparrow}$, and they can be neglected. Calculating $\langle\langle c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}a_{\mathbf{q}}\,;\,c^{+}_{\mathbf{k}\uparrow}\rangle\rangle_{+}$ in an equivalent way, and introducing the notation:

$$\begin{aligned}
&G_{m1}(\mathbf{q},\omega) = \langle\langle a_{\mathbf{q}}\,;\,a^{+}_{\mathbf{q}}\rangle\rangle \qquad ; \qquad G_{m2}(\mathbf{q},\omega) = \langle\langle a^{+}_{\mathbf{q}}\,;\,a_{\mathbf{q}}\rangle\rangle = G^{*}_{m1}(\mathbf{q},-\omega) \\
&G_{m3}(\mathbf{q},\omega) = \langle\langle a^{+}_{-\mathbf{q}}\,;\,a^{+}_{\mathbf{q}}\rangle\rangle
\end{aligned} \tag{5.7.45}$$

for the magnon Green functions determined by (5.7.25) and (5.7.33), we obtain

$$\begin{aligned}\langle\langle c_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}a^+_{-\mathbf{q}}\,;c^+_{\mathbf{k}\uparrow}\rangle\rangle_+ &= \sqrt{2J/N}\,j(-\mathbf{q}-\boldsymbol{\tau})G_\uparrow(\mathbf{k},\omega)\\ &\times\big[\{f_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}+\langle a^+_{\mathbf{q}}a_{\mathbf{q}}\rangle\}G_{m2}(\mathbf{q},\omega_1)-\langle a_{\mathbf{q}}a_{-\mathbf{q}}\rangle G_{m3}(\mathbf{q},\omega_1)\big].\end{aligned} \tag{5.7.46}$$

Defining the self-energy of the spin-up electrons by the relation

$$G_\uparrow(\mathbf{k},\omega)=\frac{1}{\hbar\omega-\varepsilon_{\mathbf{k}\uparrow}-\Sigma_\uparrow(\mathbf{k},\omega)}, \tag{5.7.47}$$

and using (3.1.10) to establish that

$$G_m(\mathbf{q},\omega)=\frac{1}{i\pi}\int\frac{G_m(\mathbf{q},\omega')}{\hbar\omega'-\hbar\omega}d(\hbar\omega'),$$

we obtain finally

$$\begin{aligned}\Sigma_\uparrow(\mathbf{k},\omega)=-\frac{2J}{N}\sum_{\mathbf{q}\boldsymbol{\tau}}|j(\mathbf{q}+\boldsymbol{\tau})|^2\frac{1}{i\pi}\int_{-\infty}^{\infty}\frac{d(\hbar\omega')}{\hbar\omega'-\hbar\omega+\varepsilon_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}}\\ \times\big[\{f_{\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}\downarrow}+\langle a^+_{\mathbf{q}}a_{\mathbf{q}}\rangle\}G_{m2}(\mathbf{q},\omega')-\langle a_{\mathbf{q}}a_{-\mathbf{q}}\rangle G_{m3}(\mathbf{q},\omega')\big].\end{aligned} \tag{5.7.48}$$

This result corresponds to that deduced by Nakajima (1967), as generalized by Fulde and Jensen (1983).

The average effective mass of the spin-up electrons at the Fermi surface is determined by

$$\frac{1}{m^*_\uparrow}=\frac{1}{\hbar^2\mathbf{k}}\frac{\partial\mathcal{E}_{\mathbf{k}\uparrow}}{\partial\mathbf{k}}\bigg|_{k=k_{F\uparrow}},$$

averaged over the direction of **k**. Here $\mathcal{E}_{\mathbf{k}\uparrow}=\varepsilon_{\mathbf{k}\uparrow}+\mathrm{Re}\big[\Sigma_\uparrow(\mathbf{k},\mathcal{E}_{\mathbf{k}\uparrow})\big]$ is the corrected energy of the spin-up electrons. We can neglect the explicit **k**-dependence of $\Sigma_\uparrow(\mathbf{k},\omega)$ in comparison to its frequency dependence, disregarding terms of the order $E_{\mathbf{q}}/\varepsilon_F$ in the derivative of $\mathcal{E}_{\mathbf{k}\uparrow}$, so that

$$\frac{\partial\mathcal{E}_{\mathbf{k}\uparrow}}{\partial\mathbf{k}}=\frac{\partial\varepsilon_{\mathbf{k}\uparrow}}{\partial\mathbf{k}}+\frac{1}{\hbar}\frac{\partial}{\partial\omega}\mathrm{Re}\big[\Sigma_\uparrow(\mathbf{k},\omega)\big]\bigg|_{\hbar\omega=\mathcal{E}_{\mathbf{k}\uparrow}}\frac{\partial\mathcal{E}_{\mathbf{k}\uparrow}}{\partial\mathbf{k}},$$

or

$$\frac{m^*_\uparrow}{m}=1-\frac{1}{\hbar}\frac{\partial}{\partial\omega}\mathrm{Re}\big[\Sigma_\uparrow(\mathbf{k}_{F\uparrow},\omega)\big]\bigg|_{\hbar\omega=\mathcal{E}_F}, \tag{5.7.49}$$

averaged over the Fermi surface. Within the same approximation, the terms in eqn (5.7.48) proportional to the magnon correlation-functions can be neglected and, to leading order, $\hbar\omega = \mathcal{E}_F$ in the ω-derivative may be replaced by $\varepsilon_{\mathbf{k}\uparrow}$, with $\mathbf{k} = \mathbf{k}_{F\uparrow}$. In the limit of zero temperature, the free-electron model then gives

$$\frac{m_\uparrow^*}{m} = 1 + \frac{2J}{N}\sum_{\mathbf{q}\boldsymbol{\tau}} |j(\mathbf{q}+\boldsymbol{\tau})|^2 \frac{1}{\pi}\int_{-\infty}^{\infty} d(\hbar\omega') \\ \times \tfrac{1}{2}\int_{-1}^{1} d\mu \frac{\mathrm{Im}\big[G_{m2}(\mathbf{q},\omega')\big]}{\big(\hbar\omega' + \Delta + \frac{(\hbar|\mathbf{q}+\boldsymbol{\tau}|)^2}{2m} - \frac{\hbar^2 k|\mathbf{q}+\boldsymbol{\tau}|}{m}\mu\big)^2},$$

subject to the conditions that $k = k_{F\uparrow}$ and $|\mathbf{k}-\mathbf{q}-\boldsymbol{\tau}| < k_{F\downarrow}$. These conditions imply that $k_{F\uparrow} - k_{F\downarrow} < |\mathbf{q}+\boldsymbol{\tau}| < k_{F\uparrow} + k_{F\downarrow}$, and that the lower bound -1 of the μ-integral is replaced by $(\hbar^2 q^2 + 2m\Delta)/(2\hbar^2 k_{F\uparrow}|\mathbf{q}+\boldsymbol{\tau}|)$. Because $\mathrm{Im}\big[G_{m2}(\mathbf{q},\omega')\big]$ is odd in ω', the contribution due to the upper bound in the μ-integral can be neglected (it is of the order $\hbar\omega'/\varepsilon_F$). Since

$$\frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\mathrm{Im}\big[G_{m2}(\mathbf{q},\omega')\big]}{\hbar\omega'} d(\hbar\omega') = \mathrm{Re}\big[G_{m2}(\mathbf{q},0)\big] = -\frac{A_{\mathbf{q}}}{E_{\mathbf{q}}^2},$$

the average mass-enhancement of the spin-up electrons at the Fermi surface is

$$\frac{m_\uparrow^*}{m} = 1 + \frac{\mathcal{N}_\downarrow(\varepsilon_F)}{2k_{F\uparrow}k_{F\downarrow}} \int_{k_{F\uparrow}-k_{F\downarrow}}^{k_{F\uparrow}+k_{F\downarrow}} dq \int \frac{d\Omega_{\mathbf{q}}}{4\pi}\, q|j(\mathbf{q})|^2 \frac{2JA_{\mathbf{q}}}{E_{\mathbf{q}}^2}, \tag{5.7.50}$$

and, by symmetry, $m_\downarrow^*/m$ is given by the same expression, except that $\mathcal{N}_\downarrow(\varepsilon_F)$ is replaced by $\mathcal{N}_\uparrow(\varepsilon_F)$. We note that the mass-enhancement only depends on the static part of the susceptibility, i.e. $G_{m2}(\mathbf{q},0)$, and that the magnitude of the mass-renormalization is intimately related to the linewidth of the spin waves derived above in eqn (5.7.38). Utilizing this connection, we can write the specific heat, in the zero-temperature limit,

$$C = \frac{\pi^2}{3}k_B^2 T\Big[\mathcal{N}_\uparrow(\varepsilon_F) + \mathcal{N}_\downarrow(\varepsilon_F) + \frac{1}{N}\sum_{\mathbf{q}} \frac{2\Gamma_{\mathbf{q}}}{\pi E_{\mathbf{q}}^2}\Big]N, \tag{5.7.51}$$

where again the $\mathbf{q}$-sum only extends over the primitive Brillouin zone. With typical values of $E_{\mathbf{q}}\mathcal{N}(\varepsilon_F) \approx 0.01$ and $2\Gamma_{\mathbf{q}}/E_{\mathbf{q}} \approx 0.05$, this expression predicts a doubling of the linear term in the heat capacity due to the interaction between the conduction electrons and the spin waves, which therefore has an appreciable effect on the effective mass of the electrons near the Fermi surface. More detailed analyses (Nakajima 1967; Fulde and Jensen 1983) show that the deformation of the electronic bands is pinned to the Fermi surface, and occurs within a narrow interval with a width corresponding to the spin-wave energies. This implies that, even if the electronic energies $\varepsilon_{\mathbf{k}\sigma}$ appearing in the magnon Green-functions were replaced with $\mathcal{E}_{\mathbf{k}\sigma}$, due to higher-order processes, this modification would not be of much importance. The total electronic heat capacity is $C_e = \sum_{\mathbf{k}\sigma} \mathcal{E}_{\mathbf{k}\sigma} df_{\mathbf{k}\sigma}/dT$, when the imaginary part of the self-energy is neglected. The extra contribution due to the coupling to the spin waves is linear only at the lowest temperatures ($k_BT < 0.05E_{\mathbf{q}}$), after which it increases more rapidly than linearly to its maximum at $k_BT \simeq 0.15E_{\mathbf{q}}$. Above $k_BT \simeq 0.3E_{\mathbf{q}}$, this contribution becomes negative and finally dies out when $k_BT \approx E_{\mathbf{q}}$. This variation with temperature was described by Fulde and Jensen (1983), and has been discussed in the context of the phonon interaction by Grimvall (1981). The bosons (magnons and phonons) do not contribute directly to the linear term in the heat capacity, which is thus a characteristic phenomenon of the Fermi gas. However, the departure from the linear variation when $k_BT > 0.05E_{\mathbf{q}}$ may be influenced by the spin-wave contribution

$$\begin{aligned} C_m &= \sum_{\mathbf{q}} \frac{1}{\pi} \int_{-\infty}^{\infty} d(\hbar\omega) \frac{2\Gamma_{\mathbf{q}}(\hbar\omega)^3}{\big\{(\hbar\omega)^2 - E_{\mathbf{q}}^2(T)\big\}^2 + \big\{2\Gamma_{\mathbf{q}}\hbar\omega\big\}^2} \frac{d}{dT}\Big(\frac{1}{1-e^{-\beta\hbar\omega}}\Big) \\ &\simeq \sum_{\mathbf{q}} E_{\mathbf{q}}(T)\frac{d}{dT}\big(n_{\mathbf{q}} + \tfrac{1}{2}\big) + \frac{\pi^2}{3}k_B^2T\sum_{\mathbf{q}} \frac{2\Gamma_{\mathbf{q}}}{\pi E_{\mathbf{q}}^2}\bigg[\frac{2}{5y^2} + \frac{4}{7y^4} + \cdots\bigg]_{y=\beta E_{\mathbf{q}}/2\pi}, \end{aligned} \tag{5.7.52}$$

to first order in $\Gamma_{\mathbf{q}}/E_{\mathbf{q}}$. The first term is the RPA spin-wave contribution (5.3.3) derived before, which dominates strongly at elevated temperatures. However, in the low-temperature limit, the second term is of the same order of magnitude as the non-linear corrections to eqn (5.7.51). For comparison, the last term in this equation is multiplied by the factor $\big[1 + 3/(5y^2) + 5/(7y^4) + \cdots\big]$ when the higher-order temperature effects are included. The additional contribution due to the non-zero linewidth of the bosons is normally not considered in the literature. It may be added to the pure electronic contribution derived by Fulde and Jensen (1983), by replacing $yL'(y)$ with $2yL'(y) + L(y)$ in their eqn (17a). The mass-enhancement effect increases proportionally to the inverse of $E_{\mathbf{q}}$ ($\Gamma_{\mathbf{q}} \propto A_{\mathbf{q}}$). On the other hand, the interval in which the linear variation occurs is diminished correspondingly, requiring a more careful consideration of the higher-order modifications.

In the metals, the itinerant electrons also interact with the phonons, and this leads to an entirely equivalent enhancement of their mass. This effect has been calculated for the whole rare earth series by Skriver and Mertig (1990), who find an increase of the band mass due to coupling to the phonons of typically about 35% for the heavy elements. Assuming the different contributions to be additive, we may write the total mass-enhancement

$$\frac{m^*}{m} = 1 + \lambda_{\mathrm{tot}} = 1 + \lambda_{\mathrm{sw}} + \lambda_{\mathrm{ph}} + \lambda_{\mathrm{c}} \tag{5.7.53}$$

as a sum of contributions from the interactions with the spin waves and the phonons, and from the possible exchange and Coulomb interactions within the electron gas itself (λ_{c}). Although the different correlation effects may increase the effective mass derived from band structure calculations by a factor of two or more, it is difficult to isolate this enhancement in heat capacity measurements, because of the quite narrow temperature interval where a truly linear behaviour can be anticipated. This interval is bounded below because of the nuclear spins, which may give large contributions to the heat capacity in the mK-range. The upper bound is due partly to the higher-order temperature effects, but most importantly to the disturbance by the normal boson contributions, approximately proportional to $T^{\alpha}\exp(-E_{\mathbf{0}}/k_BT)$ and T^3 for the magnons and the phonons respectively, which completely dominate the heat capacity at elevated temperatures. Because of this limitation, the most reliable method of determining the mass-enhancement is by measuring the temperature dependence of the dHvA effect, which also allows a separation of the contributions from the different sheets of the Fermi surface. Using this method, and comparing with the results of band structure calculations, Sondhelm and Young (1985) found values of λ_{tot} varying between 0.2 and 1.1 for Gd. The theoretical results of Fulde and Jensen (1983) lie within this range, but these measurements point to the necessity of discriminating between states of different symmetry in considering the mass-enhancement of the conduction electron gas.

5.7.3 Magnetic contributions to the electrical resistivity

The electrical resistivity of a metal can be calculated by solving the *Boltzmann equation.* We shall not discuss the theory of transport properties in detail here, but instead refer to the comprehensive treatments of Ziman (1960), and Smith and Højgaard Jensen (1989). The non-equilibrium distribution function $g_{\mathbf{k}\sigma}$, generated by the application of an external electric field $\mathbf{E}$, is written in terms of the equilibrium distribution function, and is determined by the Boltzmann equation:

$$g_{\mathbf{k}\sigma} = f_{\mathbf{k}\sigma} + f_{\mathbf{k}\sigma}(1 - f_{\mathbf{k}\sigma})\psi_{\mathbf{k}\sigma}, \quad \text{where} \quad \frac{\partial g_{\mathbf{k}\sigma}}{\partial \mathbf{k}} \cdot \frac{d\mathbf{k}}{dt} = \frac{dg_{\mathbf{k}\sigma}}{dt}\bigg|_{\mathrm{coll}}. \tag{5.7.54}$$

The electrical current-density is then determined as

$$\mathbf{j} = \overline{\overline{\sigma}} \cdot \mathbf{E} = -\frac{e}{V}\sum_{\mathbf{k}\sigma} \mathbf{v}_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma}(1 - f_{\mathbf{k}\sigma})\psi_{\mathbf{k}\sigma},$$

with $\hbar\mathbf{v}_{\mathbf{k}\sigma} = \partial\varepsilon_{\mathbf{k}\sigma}/\partial\mathbf{k}$. In the linear regime, the left-hand side of the Boltzmann equation is

$$\frac{\partial g_{\mathbf{k}\sigma}}{\partial\mathbf{k}}\cdot\frac{d\mathbf{k}}{dt} \simeq -\frac{\partial f_{\mathbf{k}\sigma}}{\partial\varepsilon_{\mathbf{k}\sigma}}e\mathbf{v}_{\mathbf{k}\sigma}\cdot\mathbf{E} = e\beta f_{\mathbf{k}\sigma}(1-f_{\mathbf{k}\sigma})\mathbf{v}_{\mathbf{k}\sigma}\cdot\mathbf{E}.$$

The collision term on the right-hand side is

$$\left.\frac{dg_{\mathbf{k}\sigma}}{dt}\right|_{\mathrm{coll}} = \sum_{\mathbf{k}'\sigma'}\big[g_{\mathbf{k}'\sigma'}(1-g_{\mathbf{k}\sigma})W(\mathbf{k}'\sigma',\mathbf{k}\sigma) - g_{\mathbf{k}\sigma}(1-g_{\mathbf{k}'\sigma'})W(\mathbf{k}\sigma,\mathbf{k}'\sigma')\big],$$

where $W(\mathbf{k}\sigma,\mathbf{k}'\sigma')$ is the probability per unit time for an electronic transition from an occupied state $|\mathbf{k}\sigma\!>$ to an unoccupied state $|\mathbf{k}'\sigma'\!>$. Linearizing the collision term, and using the principle of detailed balance, so that this term must vanish if $g_{\mathbf{k}\sigma} = f_{\mathbf{k}\sigma}$, we may reduce the Boltzmann equation to

$$e\beta f_{\mathbf{k}\sigma}(1-f_{\mathbf{k}\sigma})\mathbf{v}_{\mathbf{k}\sigma}\cdot\mathbf{E} = -\sum_{\mathbf{k}'\sigma'}(1-f_{\mathbf{k}\sigma})f_{\mathbf{k}'\sigma'}W(\mathbf{k}'\sigma',\mathbf{k}\sigma)\big(\psi_{\mathbf{k}\sigma}-\psi_{\mathbf{k}'\sigma'}\big).$$

It is possible to find an upper bound on the resistivity from this equation, with the use of a variational principle. Defining $\hat{\mathbf{u}}$ to be a unit vector along one of the principal axes of the resistivity tensor,

$$\rho_{uu} \le \frac{V}{2\beta e^2}\frac{\sum_{\mathbf{k}\sigma}\sum_{\mathbf{k}'\sigma'}(1-f_{\mathbf{k}'\sigma'})f_{\mathbf{k}\sigma}W(\mathbf{k}\sigma,\mathbf{k}'\sigma')\big(\phi_{\mathbf{k}\sigma}-\phi_{\mathbf{k}'\sigma'}\big)^2}{\big[\sum_{\mathbf{k}\sigma}\mathbf{v}_{\mathbf{k}\sigma}\cdot\hat{\mathbf{u}}\,(1-f_{\mathbf{k}\sigma})f_{\mathbf{k}\sigma}\,\phi_{\mathbf{k}\sigma}\big]^2}, \tag{5.7.55}$$

where $\phi_{\mathbf{k}\sigma}$ is an arbitrary trial function, and where the equality applies if $\phi_{\mathbf{k}\sigma} = \psi_{\mathbf{k}\sigma}$. In the case of the free-electron model, the Boltzmann equation possesses an exact solution, $\psi_{\mathbf{k}\sigma} \propto \mathbf{k}\cdot\hat{\mathbf{u}}$, if the scattering is purely elastic. As discussed, for instance, by Hessel Andersen *et al.* (1980), this trial function is still useful for treating possible inelastic scattering mechanisms, at least as long as the resistivity is dominated by elastic impurity scattering, so we shall use $\phi_{\mathbf{k}\sigma} = \mathbf{k}\cdot\hat{\mathbf{u}}$.

In the Born approximation, the transition probability per unit time is given by the Golden Rule (4.1.1), which we may here write

$$W(\mathbf{k}\sigma,\mathbf{k}'\sigma') = \frac{2\pi}{\hbar}\sum_{if}P_i|\!<\!\mathbf{k}\sigma;i\,|\,\mathcal{H}_{\mathrm{int}}\,|\,\mathbf{k}'\sigma';f\!>\!|^2\delta(\hbar\omega+E_i-E_f),$$

where $\hbar\omega = \varepsilon_{\mathbf{k}\sigma}-\varepsilon_{\mathbf{k}'\sigma'}$. Instead of basing the derivation of the magnetic resistivity on the linearized spin-wave expression (5.7.20) for $\mathcal{H}_{\mathrm{int}}$, we shall be somewhat more general and use $\mathcal{H}_{sf}$ from eqn (5.7.6) as the interaction Hamiltonian. We assume that the system is uniform, paramagnetic or ferromagnetically ordered, continue to utilize the simple free-electron model, and replace $(g-1)I(n'\mathbf{k}', n\mathbf{k})$ by $j(\mathbf{k}'-\mathbf{k}+\boldsymbol{\tau})$. The MF part (5.7.7) of the Hamiltonian may lead to a modification $\varepsilon_{\mathbf{k}\sigma} \rightarrow \widetilde{\varepsilon}_{\mathbf{k}\sigma}$ of the electronic band-states, but we can neglect this difference to leading order, and since the MF Hamiltonian does not lead to transitions between electronic states, we can replace J_{iz} by $\hat{J}_{iz} = J_{iz} - \langle J_z \rangle$ in $\mathcal{H}_{\text{int}}$, and obtain

$$
\begin{aligned}
W(\mathbf{k}\sigma, \mathbf{k}'\sigma') = \int_{-\infty}^{\infty} & d(\hbar\omega)\delta(\hbar\omega - \varepsilon_{\mathbf{k}\sigma} + \varepsilon_{\mathbf{k}'\sigma'}) \\
\times \frac{2\pi}{\hbar} \sum_{if} P_i \frac{1}{N^2} & \sum_{jj'} |j(\mathbf{k}' - \mathbf{k})|^2 e^{-i(\mathbf{k}'-\mathbf{k})\cdot(\mathbf{R}_j - \mathbf{R}_{j'})} \\
\times \Big\{ <i\,|J_{j'}^-|\,f><f\,|J_j^+|\,i>\, & \delta_{\sigma\uparrow}\delta_{\sigma'\downarrow} + <i\,|J_{j'}^+|\,f><f\,|J_j^-|\,i>\, \delta_{\sigma\downarrow}\delta_{\sigma'\uparrow} \\
& + <i\,|\hat{J}_{j'z}|\,f><f\,|\hat{J}_{jz}|\,i>\, (\delta_{\sigma\uparrow}\delta_{\sigma'\uparrow} + \delta_{\sigma\downarrow}\delta_{\sigma'\downarrow}) \Big\} \delta(\hbar\omega + E_i - E_f),
\end{aligned}
\tag{5.7.56}
$$

accounting explicitly for the condition on $\hbar\omega$ by the integral over the first δ-function. Using the same procedure as in the calculation of the neutron-scattering cross-section, when going from (4.1.16) to (4.2.1–3), we may write this:

$$
\begin{aligned}
W(\mathbf{k}\sigma, \mathbf{k}'\sigma') = & \frac{2}{N\hbar} \int_{-\infty}^{\infty} d(\hbar\omega)\delta(\hbar\omega - \varepsilon_{\mathbf{k}\sigma} + \varepsilon_{\mathbf{k}'\sigma'}) \frac{1}{1 - e^{-\beta\hbar\omega}} |j(\mathbf{k} - \mathbf{k}')|^2 \\
& \times \big\{ \chi''_{-+}(\mathbf{k} - \mathbf{k}', \omega)\delta_{\sigma\uparrow}\delta_{\sigma'\downarrow} + \chi''_{+-}(\mathbf{k} - \mathbf{k}', \omega)\delta_{\sigma\downarrow}\delta_{\sigma'\uparrow} \\
& \qquad + \chi''_{zz}(\mathbf{k} - \mathbf{k}', \omega)(\delta_{\sigma\uparrow}\delta_{\sigma'\uparrow} + \delta_{\sigma\downarrow}\delta_{\sigma'\downarrow}) \big\}.
\end{aligned}
$$

Introducing this expression into (5.7.55), and using $\phi_{\mathbf{k}\sigma} = \mathbf{k} \cdot \hat{\mathbf{u}}$ and $\mathbf{k}' = \mathbf{k} - \mathbf{q} - \boldsymbol{\tau}$, we proceed as in the derivation of eqn (5.7.36) for $\mathrm{Im}\big[\chi^{+-}_{\text{c.el.}}(\mathbf{q}, \omega)\big]$, obtaining

$$
\begin{aligned}
& \frac{1}{N} \sum_{\mathbf{k}} f_{\mathbf{k}\downarrow}(1 - f_{\mathbf{k}-\mathbf{q}\uparrow})\delta(\hbar\omega - \varepsilon_{\mathbf{k}\downarrow} + \varepsilon_{\mathbf{k}-\mathbf{q}\uparrow}) = \\
& \frac{V}{N(2\pi)^2} \int_0^\infty dk\, k^2 \int_{-1}^1 d\mu f(\varepsilon_{\mathbf{k}\downarrow}) \big\{ 1 - f(\varepsilon_{\mathbf{k}\downarrow} - \hbar\omega) \big\} \delta\big(\hbar\omega - \Delta + \varepsilon_q - \mu \frac{\hbar^2 qk}{m}\big) \\
& \quad = \frac{V}{N(2\pi)^2} \int_{\frac{\Delta}{2}}^{\infty} d\varepsilon \, \frac{m^2}{\hbar^4 q} f(\varepsilon) \big\{ 1 - f(\varepsilon - \hbar\omega) \big\} \; = \; \frac{V}{N(2\pi)^2} \frac{m^2}{\hbar^4 q} \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1},
\end{aligned}
$$

where $k_{F\uparrow} - k_{F\downarrow} < q < k_{F\uparrow} + k_{F\downarrow}$ (when $k_B T \ll \varepsilon_F$). The denominator in (5.7.55) may be calculated in a straightforward fashion and is $[N\nu/(\hbar\beta)]^2$, and we finally obtain the following expression for the resistivity, or rather its upper limit:

$$\rho_{uu}(T) \simeq \rho_0 \frac{3}{(4k_{F\uparrow}k_{F\downarrow})^2 \overline{j_u^2}} \int_{k_{F\uparrow}-k_{F\downarrow}}^{k_{F\uparrow}+k_{F\downarrow}} dq \int \frac{d\Omega_{\mathbf{q}}}{4\pi} \int_{-\infty}^{\infty} d(\hbar\omega) \\ \times |j(\mathbf{q})|^2 \big(\mathbf{q}\cdot\hat{\mathbf{u}}\big)^2 q \frac{\beta\hbar\omega}{\sinh^2(\beta\hbar\omega/2)} \frac{1}{\pi} \sum_\alpha \chi''_{\alpha\alpha}(\mathbf{q},\omega), \qquad (5.7.57a)$$

where

$$\rho_0 = \frac{3}{2}\frac{V}{N}\frac{\pi m}{\hbar e^2 \varepsilon_F}\overline{j_u^2} = \frac{m}{ne^2}\frac{\pi}{\hbar}\{\mathcal{N}_\uparrow(\varepsilon_F)+\mathcal{N}_\downarrow(\varepsilon_F)\}\overline{j_u^2}, \qquad (5.7.57b)$$

$n = \nu N/V$ is the electron density, and

$$\overline{j_u^2} = 4\frac{3}{(2k_F)^4}\int_0^{2k_F} dq \int \frac{d\Omega_{\mathbf{q}}}{4\pi}|j(\mathbf{q})|^2 \big(\mathbf{q}\cdot\hat{\mathbf{u}}\big)^2 q. \qquad (5.7.57c)$$

For cubic symmetry, ρ_{uu} is independent of u and $\big(\mathbf{q}\cdot\hat{\mathbf{u}}\big)^2$ can be replaced by $q^2/3$. In the high-temperature limit, we have

$$\frac{1}{\pi}\int_{-\infty}^{\infty} d(\hbar\omega)\frac{\beta\hbar\omega}{\sinh^2(\beta\hbar\omega/2)}\sum_\alpha \chi''_{\alpha\alpha}(\mathbf{q},\omega) \simeq \\ \frac{1}{\pi}\int_{-\infty}^{\infty} d(\hbar\omega)\frac{4}{\beta\hbar\omega}\sum_\alpha \chi''_{\alpha\alpha}(\mathbf{q},\omega) = \frac{4}{\beta}\sum_\alpha \chi'_{\alpha\alpha}(\mathbf{q},0) = 4J(J+1),$$

recalling that $\chi'_{\alpha\alpha}(\mathbf{q},0) = \frac{1}{3}\beta J(J+1)$ in this limit. This result shows that the magnetic resistivity saturates at temperatures which are so high that the ions are uniformly distributed over the states in the ground-state J-multiplet, since the condition $k_BT \ll \varepsilon_F$ is always satisfied:

$$\rho_{uu}(T) \rightarrow J(J+1)\,\rho_0 \qquad \text{for} \quad T\rightarrow\infty, \qquad (5.7.58)$$

and $J(J+1)\,\rho_0$ is called the saturation value of the *spin-disorder* resistivity. Since ρ_0 contains the factor $(g-1)^2$, the spin-disorder resistivity is proportional to the de Gennes factor, as observed (Legvold 1972). If the crystal-field splitting of the energy levels is neglected, this factor also determines the relative magnitudes of the contributions of magnetic rare earth-impurities to the resistivity of a non-magnetic host (Kasuya 1959). However, in analysing the measurements of Mackintosh and Smidt (1962) of the resistivity changes produced by small amounts of heavy rare earths in Lu, Hessel Andersen (1979) found that such crystal-field effects are indeed important at 4 K.

In a metal, the total collision rate $W(\mathbf{k}\sigma, \mathbf{k}'\sigma')$ in eqn (5.7.55) is actually the sum of contributions from several scattering mechanisms. If the trial function for elastic impurity-scattering still leads to a result reasonably close to that determined by the exact solution of the Boltzmann equation, then (5.7.55) implies that the different scattering mechanisms contribute additively to the total resistivity, in accordance with *Matthiessen's rule*:

$$\rho_{\text{total}}(T) = \rho_{\text{imp}} + \rho_{\text{m}}(T) + \rho_{\text{ph}}(T). \tag{5.7.59}$$

Here ρ_{imp} is the residual resistivity due to elastic scattering of the electrons from impurities and from lattice defects. $\rho_{\text{m}}(T)$ is the contribution, calculated above, due to the magnetic excitations, whereas $\rho_{\text{ph}}(T)$ is the equivalent term due to the phonons. The two last terms, associated with the excitations in the metal, vanish in the limit of zero temperature, so that $\rho_{\text{total}}(T = 0) = \rho_{\text{imp}}$. The problem of distinguishing between the magnetic and phonon scattering can be approximately solved by estimating the latter from the temperature dependence of the resistivity of Lu, which has an electronic structure and phonon spectrum very similar to those of the magnetic heavy rare earths, but no magnetic moment. Using this method, Mackintosh (1963) was able to show that the magnetic scattering in Tb increases as $\exp(-E_{\mathbf{0}}/k_BT)$ at low temperatures, where the spin-wave energy gap $E_{\mathbf{0}}/k_B$ was estimated to be about 20 K, a value which was subsequently verified by neutron scattering. This analysis was refined by Hessel Andersen and Smith (1979), who used the free-electron model to show that the magnetic resistivity associated with the scattering by spin waves with an isotropic dispersion relation $E_{\mathbf{q}} = E_{\mathbf{0}} + \hbar^2q^2/2m_{\text{sw}}$ is given by

$$\rho_{\text{m}}(T) = \frac{J}{4}\frac{m_{\text{sw}}^2}{m^2}\frac{E_{\mathbf{0}}k_BT}{\varepsilon_F^2}e^{-E_{\mathbf{0}}/k_BT}\big(1 + 2\frac{k_BT}{E_{\mathbf{0}}} + \tfrac{1}{2}e^{-E_{\mathbf{0}}/k_BT} + \cdots\big)\,\rho_0, \tag{5.7.60}$$

approximating the lower cut-off $k_{F\uparrow} - k_{F\downarrow}$ by 0 in (5.7.57a). A numerical calculation, utilizing the measured spin-wave energies and including one scaling parameter for the magnetic scattering and one for the phonon scattering, gave the excellent fit shown in Fig. 5.14. The disordered electric quadrupole moments of the $4f$-charge distributions can also provide a mechanism for the scattering of the conduction electrons. This is normally very difficult to distinguish from the magnetic scattering, but in TmSb, where the exchange interaction is relatively small and the electric quadrupoles large, the latter appear to dominate the electrical resistivity at low temperatures (Hessel Andersen and Vogt 1979).

Even though $k_BT \ll \varepsilon_F$, the residual resistivity ρ_{imp} is only independent of temperature as long as the ground-state properties of the

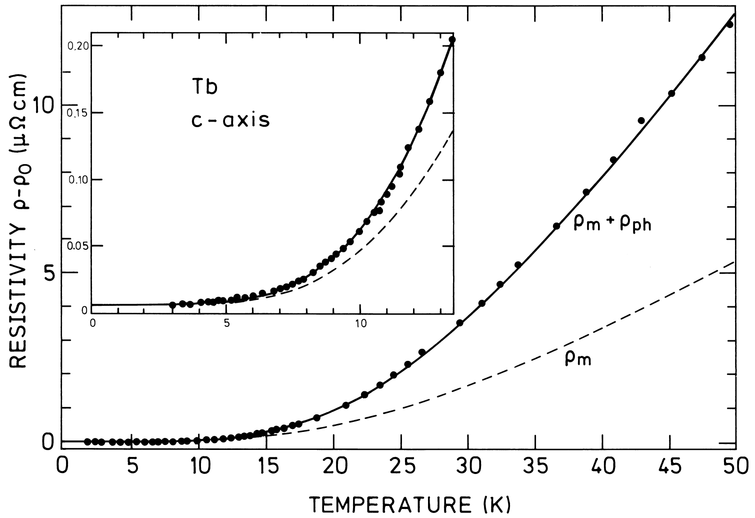

Fig. 5.14. A comparison of the measured and calculated resistivity of a Tb single crystal, as a function of temperature, after Hessel Andersen and Smith (1979). The residual resistivity has been subtracted from the experimental results. The full line includes the calculated contributions from both the magnon scattering and the phonons. The rapid increase around 20 K is predominantly due to the excitation of magnons across the energy gap.

electron gas remain unchanged. If the resistivity of the unpolarized electrons is $\rho^0_{\mathrm{total}}(T)$ and their density of states at the Fermi surface is $\mathcal{N}(\varepsilon_F)$, the polarization (5.7.16) of the conduction electrons in the ferromagnetic state leads to a scaling of the *total* resistivity, which according to eqn (5.7.55) is

$$\rho_{\mathrm{total}}(T) = \big\{1 + \zeta(T)\big\}\rho^0_{\mathrm{total}}(T) \quad ; \quad \zeta(T) = \frac{\mathcal{N}_\uparrow(\widetilde{\varepsilon}_F) + \mathcal{N}_\downarrow(\widetilde{\varepsilon}_F)}{2\mathcal{N}(\varepsilon_F)} - 1. \tag{5.7.61}$$

In $\rho^0_{\mathrm{total}}(T)$, the residual resistivity is temperature independent and the magnetic contribution is determined by the above result, if $\mathcal{N}_\sigma(\varepsilon_F)$ in (5.7.57*b*) is replaced by its paramagnetic value $\mathcal{N}(\varepsilon_F)$. The modification $\zeta(T)$, due to the polarization of the conduction electrons, depends on the temperature via the magnetization, and $\zeta(T) \propto \langle J_z \rangle^2$ at small magnetization.

The most important effect on the resistivity produced by the spin-polarization of the electronic states results from the change in the density of states at the Fermi surface, taken into account by $\zeta(T)$ in (5.7.61).

Since the other modification, the appearance of $k_{F\sigma}$ instead of the paramagnetic value k_F in (5.7.57*b*), generally only causes a minor correction to the value of the integral in this equation, the magnetic contribution to $\rho^0_{\rm total}(T)$ is approximately independent of the spin-polarization, in this model. However, the spin-polarization in the real metals may be sufficiently great to alter the topology of the Fermi surface, as discussed in Section 1.4, so that the resistivity may change abruptly with temperature or magnetic field. Under these circumstances, the resistivity must be calculated from first principles, using a realistic model of the spin-polarized energy bands. The zz-contribution should be treated separately, as the q-integral for this case should go from 0 to $2k_F$, even when the electron spins are polarized, since no spin-flip is involved in the scattering process. This modification is, however, unimportant as the dominating contributions, in the ordered phase, arise from the perpendicular spin-wave components of the susceptibility.

The above results also apply, to a good approximation, when the moments are ordered antiferromagnetically, if the value of $\zeta(T)$ is calculated for a spatial modulation of the moments. The spin-polarization of the band electrons is determined by the MF Hamiltonian, and assuming $\langle J_{iz}\rangle = \langle J_z\rangle \cos(\mathbf{Q}\cdot\mathbf{R}_i)$, we may replace (5.7.7) by

$$\begin{aligned}\mathcal{H}_{sf}(\mathrm{MF}) = -\sum_{nn'}\sum_{\mathbf{k}\mathbf{k}'}(g-1)I(n'\mathbf{k}',n\mathbf{k})\big(c^+_{n'\mathbf{k}'\uparrow}c_{n\mathbf{k}\uparrow} - c^+_{n'\mathbf{k}'\downarrow}c_{n\mathbf{k}\downarrow}\big)\\ \times\tfrac{1}{2}\big(\delta_{\mathbf{k}',\mathbf{k}+\mathbf{Q}+\boldsymbol{\tau}} + \delta_{\mathbf{k}',\mathbf{k}-\mathbf{Q}+\boldsymbol{\tau}}\big)\langle J_z\rangle,\end{aligned} \qquad (5.7.62)$$

showing that the modulated moments induce a coupling between the band electrons at the wave-vectors $\mathbf{k}$ and $\mathbf{k}\pm\mathbf{Q}+\boldsymbol{\tau}$. In the same way as the periodic lattice potential lifts the degeneracy of the band states at the Brillouin-zone boundaries (passing through $\mathbf{k}=\boldsymbol{\tau}/2$), the above MF Hamiltonian gives rise to energy gaps at the *superzone boundaries*, the planes perpendicular to, and passing through, the vectors $\mathbf{k}_s = (\pm\mathbf{Q}+\boldsymbol{\tau})/2$. If $\mathbf{k}_s$ is along the c-axis, the value of the energy gap δ is $(g-1)|I(n\mathbf{k},n-\mathbf{k})|\langle J_z\rangle$ in the nth band. The importance of the superzone gaps for the resistivity was first pointed out by Mackintosh (1962), and detailed theories were developed by Elliott and Wedgwood (1963) and Miwa (1963). These theories utilized the free-electron model and the *relaxation time* approximation, $dg_{\mathbf{k}\sigma}/dt|_{\rm coll} = -(g_{\mathbf{k}\sigma}-f_{\mathbf{k}\sigma})/\tau_{\mathbf{k}\sigma}$, giving a conductivity

$$\sigma_{uu} = \frac{e^2\beta}{V}\sum_{\mathbf{k}\sigma}\tau_{\mathbf{k}\sigma}\big(\mathbf{v}_{\mathbf{k}\sigma}\cdot\hat{\mathbf{u}}\big)^2 f_{\mathbf{k}\sigma}\big(1-f_{\mathbf{k}\sigma}\big)$$

or, if the relaxation time $\tau_{\mathbf{k}\sigma}$ is assumed to be constant over the Fermi surface,

$$\sigma_{uu} \simeq \frac{e^2\tau}{(2\pi)^3\hbar^2} \sum_\sigma \int_{\varepsilon_{\mathbf{k}\sigma}=\varepsilon_F} \left(\frac{\partial\varepsilon_{\mathbf{k}\sigma}}{\partial k_u}\right)^2 \frac{1}{|\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}\sigma}|} dS, \tag{5.7.63}$$

where dS is a surface element of the Fermi surface. Even without detailed calculations, this expression shows that the conductivity may be reduced substantially if the superzone gaps are able to eliminate significant areas of the Fermi surface. Furthermore, the Fermi-velocity factor puts different weight on the various regions of the Fermi surface in the different components of the conductivity tensor. If $\mathbf{k}_s$ is parallel to the c-axis, as in the heavy rare earths, and if its length is close to that of the Fermi wave-vector in the c-direction, only the cc-component of the conductivity is appreciably affected by the superzone boundary. For instance, an internal field of 2 kOe in the basal plane of Ho at 4 K, which eliminates the superzone energy gaps by inducing a transition from the cone to ferromagnetic ordering, increases the conductivity along the c-axis by about 30%, while decreasing the b-axis component by only about 1% (Mackintosh and Spanel 1964). As illustrated in Fig. 5.15, the anomalous increase in the resistivity in the helical phase of Tb is eliminated by a magnetic field which is large enough to suppress this structure, leaving only a weak maximum similar to that observed in Gd, which has been ascribed to critical scattering of the conduction electrons by magnetic fluctuations (de Gennes and Friedel 1958). This anomalous increase is not observed in the basal plane and the resistivity is little affected by a magnetic field (Hegland *et al.* 1963).

The theoretical calculations of the superzone effects within the free-electron model give a semi-quantitative account of the experimental observations, with a small number of adjustable parameters. For example, a superzone boundary normal to the c-axis, which intersects the Fermi surface, gives a positive contribution to $\zeta_{cc}(T)$ in (5.7.61) which is proportional to δ/ε_F, while $\zeta_{bb}(T)$ decreases like $(\delta/\varepsilon_F)^2$. Bearing in mind the analogy between the real and free-electron Fermi surfaces mentioned above, this corresponds well with the observations in, for example, Ho. In addition, the model calculations suggest that the superzone gaps are important for the value of the ordering wave-vector $\mathbf{Q}$, at which the exchange energy has its maximum (Elliott and Wedgwood 1964; Miwa 1965), by predicting a gradual reduction of the length of $\mathbf{Q}$ with the increase of the size of the superzone gaps, which are proportional to $\langle J_z \rangle$ below the Néel temperature. Hence the exchange coupling $\mathcal{J}(\mathbf{q})$ is somewhat dependent on the magnetization, because the nearly elastic intra-band contributions to the exchange interaction depend on the density of states near the Fermi surface, as is also true in the ferromagnetic case, according to (5.7.21).

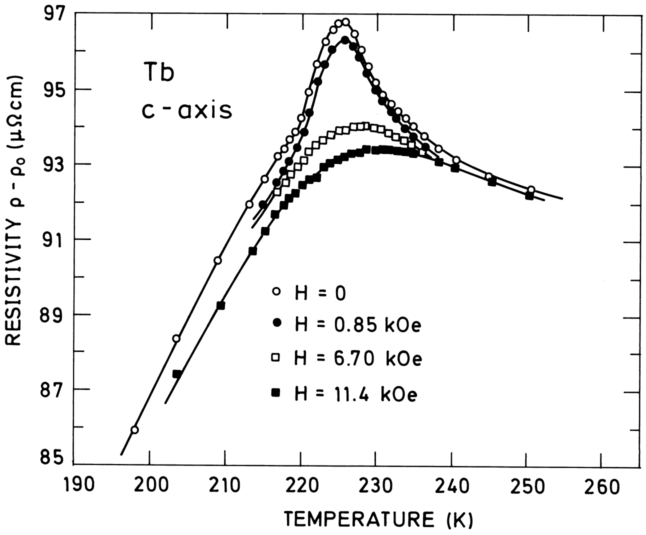

Fig. 5.15. The c-axis resistivity of Tb in the vicinity of $T_N = 230\,\mathrm{K}$, after Hegland *et al.* (1963). As the helical ordering develops, the magnetic superzones cause a sharp increase in the resistivity, which disappears at $T_C = 220\,\mathrm{K}$. The superzones may also be eliminated by a magnetic field in the b-direction, which suppresses the helical structure.

The agreement obtained between simple model calculations of the variation of $\mathbf{Q}$ and that observed experimentally is surprisingly good, to some extent fortuitously so. The band electrons are far from free-electron-like in the rare earth metals, and the approximation in which $I(n'\mathbf{k}', n\mathbf{k})$ is replaced by $j(\mathbf{k}'-\mathbf{k}+\boldsymbol{\tau})$ is rather crude. The effective free-electron model, with $j(\mathbf{q})$ proportional to a form factor $\left[1+(Aq)^2\right]^{-1}$ where $A \approx 0.2\,\text{Å}$ and $2k_F \approx 2.8\,\text{Å}^{-1}$, leads to a maximum in $\mathcal{J}(\mathbf{q})$ at $\mathbf{q} \simeq 0.3\,\text{Å}^{-1}$ parallel to the c-axis, in the paramagnetic phase. In this model, $\frac{1}{N}\sum_{\mathbf{q}} \widetilde{\mathcal{J}}(\mathbf{q})$ is found to be an order of magnitude larger than $\mathcal{J}(\mathbf{0})$, and the same is the case with the interband contributions ($\boldsymbol{\tau} \neq \mathbf{0}$) to the exchange interaction, compared to the intra-band contributions. However, various estimates indicate that all these terms are of the same order of magnitude. Lindgård *et al.* (1975) have made the only existing *ab initio* calculation of $\mathcal{J}(\mathbf{q})$ in a rare earth metal, considering the simplest case of Gd, and they obtained a reasonable account of the dependence on wave-vector, even though the magnitude differed by as much as a factor of four from that determined experimentally. Their calculations show that the exchange integral is dominated by the contributions of the *d*-like band electrons, as is the density of states at the Fermi surface. Although the effective free-electron model is not adequate for determining the exchange interaction, other quantities derived above which depend on real scattering processes close to the Fermi surface (i.e. the contributions to the spin-wave linewidths, the mass enhancement, and the resistivity), may be more trustworthy, particularly if the actual density of states of the band electrons is substituted for the free-electron value. This should especially be true for the linewidth and mass-enhancement, but the strong polarization effect (5.7.60) on the resistivity in the ferromagnetic phase, for which the maximum effect occurs in Gd, with $\zeta(T)$ approaching -0.5 in the zero temperature limit (Fulde and Jensen 1983), may be somewhat exaggerated, because the conductivity is strongly influenced by the *sp*-band electrons.