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Electrical Resistivity of Ferromagnetic Metals

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The anomalous Hall effect and the magnetoresistance of ferromagnetic metals have been investigated on the basis of the localized *d*-electron (or *f*-electron) model. The interaction between conduction electrons and the orbital angular momenta of localized electrons is taken into account. It is found that the above phenomena can be accounted for by this interaction.

The electrical resistivity of ferromagnetic metals shows an anomalous temperature dependence below the Curie temperature. This fact has been explained by Mott[1)] on the basis of the band model and by Kasuya[2)] on the basis of the localized *d*-electron model. Ferromagnetic metals also show the anomalous Hall effect and the magnetoresistance, which have been given theoretical explanations by Karplus and Luttinger[3)] and by Smit[4)], respectively, on the basis of the band model. On the other hand, the usual *s-d* interaction is isotropic and does not give rise to these effects. However, the orbital angular momenta of localized electrons remain more or less in ferromagnetic metals and we must take account of the interaction between them and conduction electrons. We shall show in this paper that the above-mentioned phenomena can be accounted for by this interaction on the basis of the localized *d*-electron model.

We shall start with the Hamiltonian

$$
\begin{aligned}
H=&\sum_{nkk'}N^{-1}e^{i(\boldsymbol{k}'-\boldsymbol{k})R_n}\\
&\times\sum_{mm'}\{(b^*_{nm+}b_{nm'+}+b^*_{nm-}b_{nm'-})\\
&\times(a^*_{\boldsymbol{k}+}a_{\boldsymbol{k}'+}+a^*_{\boldsymbol{k}-}a_{\boldsymbol{k}'-})V_{mm'}(\boldsymbol{k},\boldsymbol{k}')\\
&-(b^*_{nm+}b_{nm'+}a^*_{\boldsymbol{k}+}a_{\boldsymbol{k}'+}+b^*_{nm+}b_{nm'-}a^*_{\boldsymbol{k}-}a_{\boldsymbol{k}'+}\\
&+b^*_{nm-}b_{nm'+}a^*_{\boldsymbol{k}+}a_{\boldsymbol{k}'-}+b^*_{nm-}b_{nm'-}a^*_{\boldsymbol{k}-}a_{\boldsymbol{k}'-})\\
&\times J_{mm'}(\boldsymbol{k},\boldsymbol{k}')\}\,, \qquad (1)
\end{aligned}
$$

where

$$V_{mm'}(\boldsymbol{k},\boldsymbol{k}')=Ne^{-i(\boldsymbol{k}'-\boldsymbol{k})Rn}\iint\phi^*_{nm}(1)\phi_{\boldsymbol{k}}{}^*(2)$$
$$\times(e^2/r_{12})\phi_{nm'}(1)\phi_{\boldsymbol{k}'}(2)dv_1dv_2\,,$$
$$J_{mm'}(\boldsymbol{k},\boldsymbol{k}')=Ne^{-i(\boldsymbol{k}'-\boldsymbol{k})Rn}\iint\phi^*_{nm}(1)\phi_{\boldsymbol{k}}{}^*(2)$$
$$\times(e^2/r_{12})\phi_{\boldsymbol{k}'}(1)\phi_{nm'}(2)dv_1dv_2\,.$$

This Hamiltonian represents the interaction between conduction electrons and localized electrons. Here, $a_{\boldsymbol{k}\pm}$ is the destruction operator of a conduction electron and $b_{nm\pm}$ is that of a localized electron in the m-th state at the n-th site. V and J are Coulomb and exchange integrals, respectively. Usually, m was restricted to be equal to m'.

If the total orbital and spin angular momenta of localized electrons are good quantum numbers, we can write this expression as representing the interaction between conduction electrons and the total orbital and spin angular momenta of localized electrons. For this purpose, we have to do two things. Firstly, the $b_{nm\pm}{}^*b_{nm'\pm}$ is represented by a function of the orbital angular momentum of a localized electron. Secondly, by expanding the Bloch function in a series of

$$\phi_{\boldsymbol{k}}(\boldsymbol{r})=V^{-1/2}\Sigma_l(2\,l+1)i^lj_l(kr)P_l(\cos\theta_{kr}),\quad(2)$$

we express V and J by a power series of $\boldsymbol{k}$ and $\boldsymbol{k}'$. In the summation in Eq. (2) we restrict ourselves to the terms of $l=0$ and 1, that is, to the lowest order in which we can obtain the relevant effects.

Then we can write Eq. (1) as follows:

$$\begin{aligned}H=&-\Sigma_{n\boldsymbol{k}\boldsymbol{k}'}N^{-1}e^{i(\boldsymbol{k}'-\boldsymbol{k})Rn}a_{\boldsymbol{k}}{}^*a_{\boldsymbol{k}'}\\&\times\Sigma_{i=1}^{n_0}[R_1\{(\boldsymbol{l}_i\boldsymbol{\kappa})(\boldsymbol{l}_i\boldsymbol{\kappa}')+(\boldsymbol{l}_i\boldsymbol{\kappa}')(\boldsymbol{l}_i\boldsymbol{\kappa})\\&-2\,l(l+1)(\boldsymbol{\kappa}\boldsymbol{\kappa}')/3\}\\&+\{F_0+2F_1(\boldsymbol{\kappa}\boldsymbol{\kappa}')+(3i/2)F_2\boldsymbol{l}_i\cdot(\boldsymbol{\kappa}'\times\boldsymbol{\kappa})\\&-(F_3/2)[(\boldsymbol{l}_i\boldsymbol{\kappa})(\boldsymbol{l}_i\boldsymbol{\kappa}')+(\boldsymbol{l}_i\boldsymbol{\kappa}')(\boldsymbol{l}_i\boldsymbol{\kappa})\\&-2l(l+1)(\boldsymbol{\kappa}\boldsymbol{\kappa}')/3]\}\{1/2+2(\boldsymbol{s}_i\boldsymbol{s}_c)\}]\,,\end{aligned}\quad(3)$$

where n_0 is the number of $3d$ (or $4f$) electrons at the n-th site, $\boldsymbol{\kappa}$ and $\boldsymbol{\kappa}'$ are unit vectors in the directions of $\boldsymbol{k}$ and $\boldsymbol{k}'$, R_1 is essentially the electric quadrupole moment of the ion and F_i are the constants derived from the exchange integral. When the orbital and spin angular momenta, $\boldsymbol{l}_i$ and $\boldsymbol{s}_i$, of an individual electron are represented by total orbital and spin angular momenta, this Hamiltonian can be expressed by

$$\begin{aligned}H=&-\Sigma_{n\boldsymbol{k}\boldsymbol{k}'}N^{-1}e^{i(\boldsymbol{k}'-\boldsymbol{k})Rn}a_{\boldsymbol{k}}{}^*a_{\boldsymbol{k}'}\\&\times[c_1(R_1-F_3/4)\{(\boldsymbol{L}_n\boldsymbol{\kappa})(\boldsymbol{L}_n\boldsymbol{\kappa}')+(\boldsymbol{L}_n\boldsymbol{\kappa}')(\boldsymbol{L}_n\boldsymbol{\kappa})\\&-2L(L+1)(\boldsymbol{\kappa}\boldsymbol{\kappa}')/3\}\\&+(3i/4)F_2\boldsymbol{L}_n\cdot(\boldsymbol{\kappa}'\times\boldsymbol{\kappa})\\&+2(\boldsymbol{S}_n\boldsymbol{s}_c)\{F_0+2F_1(\boldsymbol{\kappa}\boldsymbol{\kappa}')+(3i/2)c_2F_2\boldsymbol{L}_n\cdot(\boldsymbol{\kappa}'\times\boldsymbol{\kappa})\\&-(c_3/2)F_3[(\boldsymbol{L}_n\boldsymbol{\kappa})(\boldsymbol{L}_n\boldsymbol{\kappa}')+(\boldsymbol{L}_n\boldsymbol{\kappa}')(\boldsymbol{L}_n\boldsymbol{\kappa})-2L(L+1)\\&\times(\boldsymbol{\kappa}\boldsymbol{\kappa}')/3]\}]\end{aligned}\quad(4)$$

where c_i are some numerical constants which depend on the kind of the ion. This is our basis Hamiltonian which represents the interaction between conduction electrons and orbital and spin angular momenta of localized electrons.

There are two cases in which this Hamiltonian can be further simplified. In the first place, if the orbital ground state is nondegenerate, the average of $\boldsymbol{L}$ vanishes and this Hamiltonian reduces to the usual s-d Hamiltonian, H_0. If we introduce the spin-orbit coupling, $\lambda\boldsymbol{L}\cdot\boldsymbol{S}$, we have correction terms through a perturbation procedure, which are given by

$$\begin{aligned}\mathscr{H}=&H_0+\Sigma_i\{(0|H-H_0|i)(i|H_{LS}|0)/(E_0-E_i)\\&\quad+c.c.\}\\&+\Sigma_{ii'}(0|H_{LS}|i)(i|H-H_0|i')\\&\quad\times(i'|H_{LS}|0)/(E_i-E_0)(E_{i'}-E_0)\\&+\Sigma_{ii'}\{(0|H_{LS}|i)(i|H_{LS}|i')\\&\quad\times(i'|H-H_0|0)/(E_i-E_0)(E_{i'}-E_0)\\&\quad+c.c.\}.\end{aligned}\quad(5)$$

The second term represents the process in which the orbital state of localized electrons is excited to the i-th state, while a conduction electron is scattered and then returns to the ground state through the spin-orbit interaction. We find that this term is proportional to $i(\lambda/\Delta E)(\boldsymbol{k}'\times\boldsymbol{k})\cdot\boldsymbol{S}$ and changes its sign when $\boldsymbol{k}$ and $\boldsymbol{k}'$ are interchanged. This fact becomes important when we discuss the anomalous Hall effect. Other terms correspond to higher-order processes. They are proportional to λ^2 and depend in a complicated way on the directions of initial and final wave vectors and localized spins.

In the second place where the basis Hamiltonian can be simplified, we have rare-earth metals, in which the total angular momentum $\boldsymbol{J}$ of $4f$ electrons is a good quantum number. Then our basis Hamiltonian can be represented in terms of $\boldsymbol{J}$. But we shall not present the expression here.

Now we shall calculate the electrical resistivity, regarding (5) as a perturbation on the motion of conduction electrons which causes the deviation from the periodic potential. The transition probability of a process in which a conduction electron is scattered from a state $\boldsymbol{k}$ to $\boldsymbol{k}'$ is expressed to the first Born approximation by

$$W(\boldsymbol{k},\ \boldsymbol{k}')=(2\pi/\hbar)|H_{\boldsymbol{k}.\boldsymbol{k}'}|^2\delta(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'}). \qquad (6)$$

Calculating matrix elements from (5) and solving the Boltzmann equation, we find that the resistivity can be expressed by

$$\rho=\rho_0+\rho_1(\boldsymbol{\alpha}\cdot\boldsymbol{\beta})^2+\rho_2\Sigma_{i>j}\alpha_i\alpha_j\beta_i\beta_j, \qquad (7)$$

where $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are unit vectors in the directions of the electric field and the magnetization, respectively. The first term may come from lattice scattering, impurity scattering and isotropic exchange scattering and represents the isotropic resistivity, while the second and third terms come from the correction terms to the exchange scattering and represents the anisotropic parts. Their ratios to the first term are roughly given by $\lambda^2/\Delta E^2$, which is around 10^{-2}. This magnitude is just what is observed for iron group metals and alloys.

Now we shall discuss the anomalous Hall effect. The transition probability from $\boldsymbol{k}$ to $\boldsymbol{k}'$ is equal to that from $\boldsymbol{k}'$ to $\boldsymbol{k}$ to the first Born approximation, where the probability is given by the absolute square of matrix elements, and does not lead to the anomalous Hall effect. So we must see if any term which is proportional to $\boldsymbol{k}'\times\boldsymbol{k}$ might remain to the second Born approximation, in which the transition probability is expressed by

$$\begin{aligned}W(\boldsymbol{k}',\boldsymbol{k})=&(2\pi/\hbar)\delta(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'})[H_{\boldsymbol{k}.\boldsymbol{k}'}H_{\boldsymbol{k}'.\boldsymbol{k}}\\&+\Sigma'_{\boldsymbol{k}''}\{H_{\boldsymbol{k}.\boldsymbol{k}''}H_{\boldsymbol{k}''.\boldsymbol{k}'}H_{\boldsymbol{k}'.\boldsymbol{k}}/(E_{\boldsymbol{k}}-E_{\boldsymbol{k}''}+is)\\&+c.c.\}]. \qquad (8)\end{aligned}$$

Actually we find that the probability does contain a term proportional to $\boldsymbol{k}'\times\boldsymbol{k}$.

Solving the transport equation with (8), we find that the current is expressed by

$$\boldsymbol{j}=\sigma E(\boldsymbol{\alpha}+\gamma\boldsymbol{\beta}\times\boldsymbol{\alpha})\ , \qquad (9)$$

where the second term represents the anomalous Hall current which is perpendicular both to the applied field and to the magnetization. It is convenient to discuss the effect in terms of the Hall resistivity, which is defined by

$$\rho_H=E_\perp/j_{/\!/},$$

where $j_{/\!/}$ is the component of the current density to the direction of the applied field and $E_\perp$ is the component of the electric field to the direction which is perpendicular both to the current and to the magnetization. We find

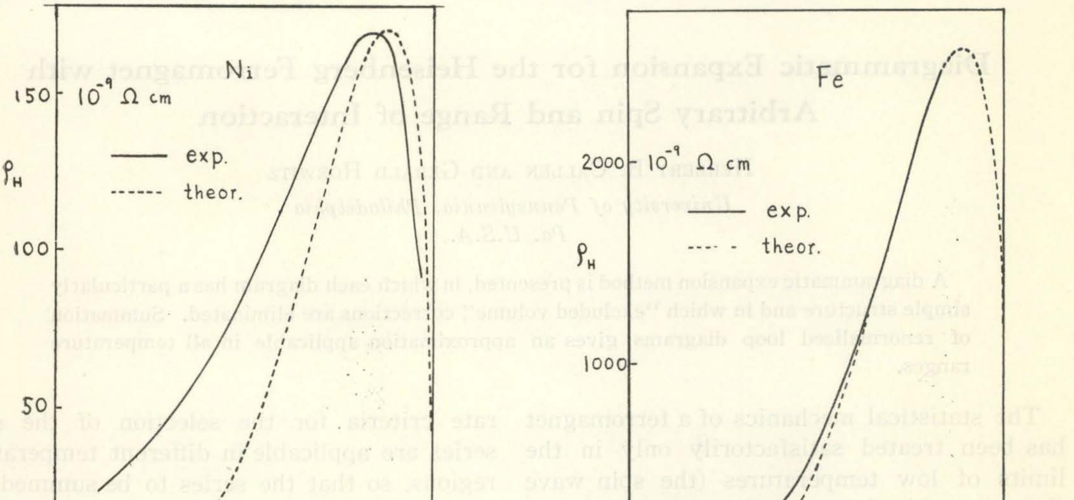

Fig. 1. Theoretical and experimental curves for the anomalous Hall resistivity of nickel and iron.

$$\rho_H=(3\lambda/\Delta E)(V/N)^2(2m^5)^{1/2}\langle(M-\langle M\rangle)^3\rangle \times F_2F_0^2/\hbar^4e^2E_F^{1/2}, \quad (10)$$

where M denotes the z component of a localized spin. The factor, $\langle(M-\langle M\rangle)^3\rangle$, represents the temperature variation of the Hall resistivity. It is remarkable that the lattice and impurity scatterings do not contribute to the Hall resistivity, although they do to the Hall conductivity. If we take

$$(\lambda/\Delta E)F_2F_0^2=-0.03\ (\mathrm{eV})^3 \quad \text{for nickel}$$
$$=\ 0.12\ (\mathrm{eV})^3 \quad \text{for iron,}$$

the agreement between (10) and experimental results[5] is such as shown in Fig. 1.

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DISCUSSION

J. ELLIOTT: Is the temperature dependence of your result the same as the ρ^2 dependence predicted by Luttinger?

J. KONDO: Incidentally it has the similar temperature dependence as that by Luttinger as long as the content of impurity atoms is small.

J. ELLIOTT: Some years ago, a student of mine, Mr. Roycroft, began a similar calculation, which was not completed. He noted that the spin orbit coupling in the conduction electrons produced an exactly similar but probably smaller matrix element.

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Diagrammatic Expansion for the Heisenberg Ferromagnet with Arbitrary Spin and Range of Interaction

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A diagrammatic expansion method is presented, in which each diagram has a particularly simple structure and in which "excluded volume" corrections are eliminated. Summation of renormalized loop diagrams gives an approximation applicable in all temperature ranges.

The statistical mechanics of a ferromagnet has been treated satisfactorily only in the limits of low temperatures (the spin wave theory) or of high temperatures (expansion in T_c/T). We here describe an approximate theory based on a new form of linked cluster expansion for spin variables, and on a partial summation of selected sub-series. Separate criteria for the selection of the sub-series are applicable in different temperature regions, so that the series to be summed are those containing all diagrams which are dominant at any temperature. The resultant theory is then approximately valid through the entire temperature range, including the particularly interesting neighborhood of the transition temperature.

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