Application of the Side-Jump Model to the Hall Effect and Nernst Effect in Ferromagnets

L. Berger
Physics Department, Carnegie-Mellon University, Pittsburgh, Pennsylvania 15213
(Received 8 June 1971)

We recently showed that an electron wave packet undergoes an abrupt, sideways jump Δy during scattering in the presence of spin-orbit interaction. This causes the Hall effect in ferromagnets around room temperature ($R_s \propto \rho^2$). The value of the side jump per collision ($\Delta y \approx 10^{-10}$ m) seems the same for impurity and phonon scattering. A more complete justification of the side-jump model is given here. This model is used to derive the isothermal Nernst coefficient Q_s^{is}, giving $Q_s^{is} \propto \rho T$, where ρ is the resistivity. If spin-disorder scattering is also introduced, then the Hall conductivity γ_{Hs} is not affected, but the Nernst coefficient becomes $Q_s^{is} = -T(\alpha + \beta\rho)$. This formula agrees with the data of Kondorskii and Vasileva on Fe, Ni, Co, Gd, and Fe-Ni. The side jump is assumed to have the same value for spin disorder as for impurity or phonon scattering. The constant α is predicted to exist even in pure metals, in agreement with the above data but not with the Kondorskii theory.

I. INTRODUCTION

The isothermal Nernst effect (often called the Ettingshausen-Nernst effect) is characterized[1] by the existence of an electric field $\vec{E}$ in a direction normal to a temperature gradient and normal to the magnetic induction $\vec{B}$. In a ferromagnet there is also[2] a contribution from the magnetization $\vec{M}$:

$$E_y = -(Q_0^{is} B_z + Q_s^{is} M_z)\frac{dT}{dx}, \tag{1}$$

where $\vec{B} \parallel \vec{M} \parallel z$, the temperature gradient is $\vec{\nabla} T \parallel x$, Q_0^{is} and Q_s^{is} are, respectively, the ordinary and extraordinary isothermal Nernst coefficients, and the electrical current density $\vec{I}$ is assumed to be zero. Saturation magnetization will be denoted by M_s. The extraordinary coefficient Q_s^{is} has probably the same origin as the extraordinary Hall coefficient R_s, and requires the existence of a spin-orbit interaction. Kondorskii[3] proposed a theory which takes into account impurity and phonon scattering, and predicts

$$Q_s^{is} = -(\alpha + \beta\rho)T, \tag{2}$$

where ρ is electrical resistivity and α and β are constant coefficients. In a very interesting paper[4] Kondorskii and Vasileva have shown[5] experimentally that Eq. (2) holds for Fe, Ni, Co, Gd, and Fe-Ni alloys, between room temperature and the neighborhood of the Curie point. However, it is not clear to what extent the Kondorskii theory is affected by a calculation error pointed out[6] in later publications.

Abelskii[7] has developed a theory which takes into account magnon scattering. He obtained

$$Q_s^{is} \propto R_s(T/\rho), \tag{3}$$

where R_s is the extraordinary Hall coefficient.

These theories are rather complicated and do not give much insight into the phenomena. Using a representation ("physical bands") which achieves maximum diagonalization of the Hamiltonian, it is possible to build a much simpler theory giving equivalent results. This has been done recently[8] by the author for the Hall effect, and the purpose of the present paper is to extend the work to the problem of the Nernst effect. It appears that the main physical mechanism responsible for the Hall and Nernst effects of ferromagnets around room temperature is the so-called "side jump" Δy performed by the electron during each collision with an impurity or phonon. This abrupt jump, of the order of $\Delta y \approx 10^{-10}$–$10^{-11}$ m, is in a direction perpendicular to the incident wave vector and to the magnetization. As we show below, the side-jump model predicts correctly Eq. (2) for Q_s^{is}.

Added to the side-jump mechanism there is also the Smit asymmetric scattering[9,10] similar to Mott scattering. It is important mostly at low temperatures, and in alloys. Meyer has proposed[11] a theory of the Nernst effect, based on the Karplus-Luttinger theory of the Hall effect of ferromagnets. In the latter theory, each Bloch wave has a periodic electric dipole moment $\vec{q}$, perpendicular to $\vec{k}$ and to the magnetization $\vec{M}$. The time variation of $\vec{k}$ caused by $\vec{E}$ implies a corresponding variation of the transverse dipole, equivalent to a current. This transverse polarization current is assumed to be the origin of the Hall effect of ferromagnets. Unfortunately, the time variation of the dipole caused by $\vec{E}$ must be exactly canceled[12(a)] in the stationary state by the decelerating effect of phonon and impurity scattering. The only effects which do not cancel out are our side jump and asymmetric scattering (see Appendix B).

II. JUSTIFICATION OF SIDE-JUMP MODEL

The existence and value of the abrupt sideways jump Δy, undergone by a wave packet on scattering by an impurity (or phonon), was derived in an earlier publication by the author,[8] using partial-wave

methods or the first Born approximation. As far as the author knows, this effect had not been treated before in the large literature on quantum scattering theory. Using the side-jump concept, a nonclassical transport theory of great simplicity was constructed by the author. The key to the simplicity of the theory was the fact that the Hamiltonian H_p of the periodic lattice was completely diagonalized, including the effects of interband mixing by spin-orbit interaction and by the applied electric field. In the H_p representation, all nonclassical contributions to the extraordinary Hall effect, such as the nonclassical side-jump current $\vec{J}$, are localized inside the impurities. Note that $\vec{J}$ represents a time variation of the usual Wannier coordinate $\vec{R}$, and not of the transverse dielectric polarization $\vec{q}$; it is the behavior of $\vec{R}$ alone which can be calculated by free-electron scattering methods.

A short discussion of other proposed mechanisms for the Hall effect of ferromagnets was given in the author's earlier paper.[8] In view of the divergent opinions expressed in the literature, we want here to expand this discussion.

The classical current $\vec{j} = \hbar^{-1} e \sum_k f_k \partial E_k / \partial \vec{k}$ is not localized in the impurities. It arises from the field $\vec{E}$ pushing the distribution f_k of Bloch waves away from equilibrium. This process is limited by scattering. If the differential scattering cross section has a left-right asymmetry, f_k will be modified in such a way that the electron gas will acquire a transverse $\vec{j}$ component (Smit[9] asymmetric scattering, mentioned above).

Considering now the acceleration itself of the electron by $\vec{E}$, $d\vec{k}/dt$ can be shown[12(b)] to be exactly parallel to $\vec{E}$ in the periodic lattice, as for free electrons. However, Doniach[12(c)] and Fivaz[12(d)] have suggested that the action of $\vec{E}$ during the process of impurity scattering itself would accelerate the electron in a direction at an angle to $\vec{E}$. This effect, called "anomalous driving term," would be formally equivalent to the electronic charge being a tensor rather than a scalar. This would provide a second mechanism for a transverse component of $\vec{j}$. In our earlier paper, we sketched a proof that such a mechanism does not exist. We give a more complete proof in Appendix A, in the first Born approximation. A somewhat similar conclusion (nonexistence of a "field term") is reached by other authors.[6]

A last possibility would involve $\vec{E}$ creating a nonclassical current $\vec{J}$ in the impurities by direct polarization of the impurity wave functions, as represented by the tensor $\overleftrightarrow{\Sigma}$:

$$\vec{J} = (s\Delta y/v)(j \times \alpha) + \overleftrightarrow{\Sigma} \cdot \vec{E}\,, \quad \vec{\alpha} = \vec{M}/M_s$$

while the first term represents our $\vec{j}$-dependent side-jump current [which agrees with Eq. (26) of Ref. 8]. However, if we surround the impurity atom tightly with a spherical boundary, it is obvious that such a localized part of the wave function will, for given boundary condition and surroundings, usually have a discrete, atomiclike spectrum with energy gaps of order ≈ 1 eV, and is very rigid against field polarization. It is much easier for $\vec{E}$ to polarize the remaining periodic part of the lattice which has an almost-degenerate spectrum, thus creating the classical current $\vec{j}$; this will change in turn the impurity wave function through the boundary condition and polarize the impurity indirectly, as described by the first term of the equation above (side-jump current). This argument, which can be written more explicitly, suggests strongly that the ($\vec{j}$-dependent) side-jump mechanism is much more effective than this $\vec{E}$-dependent impurity-polarization effect. Moreover, this direct impurity-polarization effect would predict for the Hall resistivity $\rho_H \propto \rho^3$, while $\rho_H \propto \rho^2$ is observed.

An important by-product of the scattering calculation of Appendix A is the idea that the side jump Δy may also be described as a left-right asymmetry of Δt_L. The delay time Δt_L is the time after which the scattered wave packet emerges from the impurity.

Finally, we give a complete accounting of all currents existing in a ferromagnet (see Appendix B). The conclusion of this accounting is that, because of certain cancellations already noted by Smit,[12(a)] only the classical Smit asymmetric scattering current $\vec{j}$ and the nonclassical side-jump current $\vec{J}$ actually exist. The fact that the side-jump current $\vec{J}$, located in impurities, was not included in the considerations of Smit[9,12(a)] is at the origin of the discrepancy between his conclusions and those of Luttinger[12(e)] or of Adams and Blount.[12(f)]

III. PELTIER TENSOR

The electrical conductivity tensor $\overleftrightarrow{\sigma}$ and the Peltier tensor $\overleftrightarrow{\pi}$ of an isothermal metal are defined by[1,13]

$$\vec{q} = \overleftrightarrow{\pi} \cdot \vec{I} = \int \frac{\epsilon_e - \epsilon_F^e}{e_e} \frac{d\vec{I}_e}{d\epsilon_e} d\epsilon_e + \int \frac{\epsilon_h - \epsilon_F^h}{\epsilon_h} \frac{d\vec{I}_h}{d\epsilon_h} d\epsilon_h\,, \tag{4}$$

$$\vec{I} = \overleftrightarrow{\sigma} \cdot \vec{E}\,, \tag{5}$$

where ϵ_e, ϵ_h are the energies of electrons and holes. The Fermi levels are $\epsilon_F = \epsilon_F^e = -\epsilon_F^h$. Writing the charges $e_h = -e_g = e$, we obtain the Mott relation[13]

$$\overleftrightarrow{\pi} = -\frac{\pi^2}{3} \frac{k_B^2}{e} T^2 \left(\frac{d}{d\epsilon_F} \overleftrightarrow{\sigma} \right) \cdot \overleftrightarrow{\sigma}^{-1}\,, \tag{6}$$

where $e = 1.6 \times 10^{-19}$ C.

Isolating the antisymmetric part $\overleftrightarrow{\rho}_a$ of the resistivity tensor $\overleftrightarrow{\rho} = \overleftrightarrow{\sigma}^{-1}$ and the scalar resistivity ρ, we write

$$\overleftrightarrow{\rho} = \rho \overleftrightarrow{1} + \overleftrightarrow{\rho}_a . \tag{7}$$

If the second term of Eq. (7) is much smaller than the first one, we obtain finally for the nonzero off-diagonal elements

$$\pi_{yx} = -\pi_{xy} = \frac{\pi^2}{3} \frac{k_B^2}{e} T^2 \frac{d}{d\epsilon_F} (\tan\phi_H) , \tag{8}$$

where $\tan\phi_H = \rho_{yx}/\rho$ is the tangent of the Hall angle, while the diagonal element is as expected[13]

$$\pi_{xx} = \pi_{yy} = \pi_{zz} = \frac{\pi^2}{3} \frac{k_B^2}{e} T^2 \frac{d}{d\epsilon_F} (\ln\rho) . \tag{9}$$

IV. ISOTHERMAL NERNST EFFECT

The thermoelectric tensor $\overleftrightarrow{\mu}$ is defined by

$$\vec{E}^* = \overleftrightarrow{\mu} \cdot \vec{\nabla} T , \tag{10}$$

where $\vec{I} = 0$ is assumed to hold. The "electrochemical field" is defined by $\vec{E}^* = \vec{E} + \vec{\nabla}\epsilon_F/e$, where $e = 1.6 \times 10^{-19}$ C. It is well known[1,13] that most electrical measuring instruments measure $\vec{E}^*$ rather than $\vec{E}$. $\overleftrightarrow{\mu}$ is related to the Peltier tensor by the Kelvin relation[1,13]

$$\overleftrightarrow{\mu} = \overleftrightarrow{\pi}/T . \tag{11}$$

The isothermal Nernst electric field of Eq. (1) may be related to $\overleftrightarrow{\mu}$ or $\overleftrightarrow{\pi}$:

$$E_y = E_y^* = \mu_{yx} \frac{dT}{dx} = \frac{\pi_{yx}}{T} \frac{dT}{dx} . \tag{12}$$

Combining Eqs. (1), (8), and (12), we obtain

$$Q_s^{is} = \frac{1}{M_s} \frac{\pi^2}{3} \frac{k_B^2}{e} T \frac{d}{d\epsilon_F} (\tan\phi_{Hs}) , \tag{13}$$

where $\tan\phi_{Hs}$ is the extraordinary part of $\tan\phi_H$, which depends on the magnetization $\vec{M}$ rather than on the field $\vec{B}$.

The general relation of Eq. (13), which does not seem to have been noticed before, could also be written in a similar manner between the ordinary coefficient Q_0^{is} and $\tan\phi_{H0}$, where ϕ_{H0} is the ordinary part of the Hall angle.

V. SIDE JUMP AND ASYMMETRIC SCATTERING IN PRESENCE OF IMPURITIES

The Hall angle of a ferromagnetic metal has been calculated[8] in the case of the side-jump mechanism. Then, for a two-band model, Eq. (13) becomes, in the low-field limit, $\omega_c\tau \ll 1$, if $\vec{M} \parallel z$:

$$Q_s^{is} = \frac{1}{M_s} \frac{\pi^2}{3} \frac{k_B^2}{e} T \frac{d}{d\epsilon_F} \left(\frac{\sigma_e(\Delta y_e/\Lambda_e) + \sigma_h(\Delta y_h/\Lambda_h)}{\sigma_e + \sigma_h} \right) \tag{14a}$$

$$= \frac{1}{M_s} \frac{\pi^2}{3} \frac{k_B^2}{e} T \frac{d}{d\epsilon_F} \left(\frac{(n_e e_e^2 \Delta y_e/\hbar k_e) + (n_h e_h^2 \Delta y_h/\hbar k_h}{\sigma_e + \sigma_h} \right), \tag{14b}$$

where $\sigma_e = n_e e_e^2/m_e s_e$, $\sigma_h = n_h e_h^2/m_h s_h$ are the conductivities of the electron and hole bands, Δy_e, Λ_y and Λ_e, Λ_k are, respectively, the side jumps and the mean free paths of electrons and holes, and s_e, s_h are their relaxation frequencies.

For a given value of Δy_e and Δy_h (scattering dominated by a given kind of impurity), Eqs. (14) imply

$$Q_s^{is} \propto T^1 \rho^1 . \tag{15}$$

Physically, it can be said that the extraordinary Nernst effect arises because electrons of different energies undergo side jumps of different magnitude. As a result, the side jumps of energetic electrons diffusing down the temperature gradient do not quite cancel the side jumps of less energetic electrons diffusing up the temperature gradient. Thus a net transverse electric current tends to appear, resulting in an excess of electronic charge on one side of the sample, and in the existence of the transverse Nernst electric field.

The Hall angle of a ferromagnet has also been calculated[10] in the case of the asymmetric-scattering mechanism. For a two-band model, Eq. (13) becomes, in the low-field limit,

$$Q_s^{is} = \frac{1}{M_s} \frac{\pi^2}{3} \frac{k_B^2}{e} T \frac{d}{d\epsilon_F} \left(-\frac{\sigma_e(s_{xy}^e/s_{xx}^e) + \sigma_h(s_{xy}^h/s_{xx}^h)}{\sigma_e + \sigma_h} \right) , \tag{16}$$

where the tensors $\overleftrightarrow{s}^e$ and $\overleftrightarrow{s}^h$ have the dimension of a relaxation frequency. The diagonal elements $s_{xx}^e = s_{yy}^e = s_{zz}^e$ represent the usual relaxation frequency and are proportional to the impurity concentration c. The off-diagonal elements $s_{xy}^e = -s_{yx}^e$ describe[10] the asymmetric scattering of electrons on impurities, and are proportional to M_z and to c. If the scattering is dominated by one kind of impurity, then Eq. (16) implies

$$Q_s^{is} \propto T^1 \rho^0 . \tag{17}$$

The side-jump model predicts[8] $R_s \propto \rho^2$, while asymmetric scattering[10] gives $R_s \propto \rho$. Then we see that Eqs. (15) and (17) both lead to Eq. (3), written originally by Abelskii for magnon scattering rather than for impurity scattering.

VI. COMBINED IMPURITY AND PHONON SCATTERING

As was mentioned in an earlier publication, [8] the fact that the value of the side jump Δy is theoretically found to be rather insensitive to the depth, sign, and range of a central impurity potential suggests that the same constant Δy value might apply even in the case of the (noncentral) deformation potential which describes phonon-electron interaction. This idea is in good agreement[8] with existing data for dilute Fe alloys around room temperature, which show that phonons and various impurities have the

same influence on the extraordinary Hall effect. We will show, however, that they do not have the same influence on the extraordinary Nernst effect.

Equation (13) may be written in the form

$$Q_s^{is} = \frac{1}{M_s}\,\frac{\pi^2}{3}\,\frac{k_B^2}{e}\,T\,\frac{d}{d\epsilon_F}\,(\gamma_{Hs}\rho)\,. \tag{18}$$

If we use a one-band model, the expressions for the extraordinary Hall conductivity γ_{Hs} and the scalar resistivity ρ are $\gamma_{Hs} = \Delta y\, n e^2/\hbar k$ and $\rho = 1/\sigma = ms/ne^2$.

Writing $s = s^i + s^{ph}$, where i and ph stand for impurity and phonon, Eq. (18) becomes

$$Q_s^{is} = -T(\alpha + \beta\rho)\,,$$

$$\alpha = -\frac{1}{M_s}\,\frac{\pi^2}{3}\,\frac{k_B^2}{e}\,\frac{r_i - r_{ph}}{\epsilon_F}\,\rho_i\,\gamma_{Hs}\,, \tag{19}$$

$$\beta = -\frac{1}{M_s}\,\frac{\pi^2}{3}\,\frac{k_B^2}{e}\left[\frac{d}{d\epsilon_F}\,\gamma_{Hs} + \left(\frac{\gamma_{Hs}}{\epsilon_F}\right)(r_{ph} - r_n)\right], \tag{20}$$

where

$$r_n = \frac{\epsilon_F}{n}\,\frac{dn}{d\epsilon_F}\,, \qquad r_{ph} = \frac{\epsilon_F}{s^{ph}}\,\frac{ds^{ph}}{d\epsilon_F}\,, \qquad r_i = \frac{\epsilon_F}{s^i}\,\frac{ds^i}{d\epsilon_F}\,,$$

and ρ_i is the impurity resistivity:

$$\rho_i = ms^i/ne^2\,.$$

The coefficients α and β are temperature independent. Thus we have obtained a prediction agreeing with Eq. (2). Nevertheless, Eq. (19) leads to serious difficulties in the case of pure iron or gadolinium, which exhibit[4] a large α value even though ρ_i should be quite small in a pure metal. Kondorskii's theory[3] leads to the same inconsistency, too. We will present in Sec. VII a more satisfactory theory, based on spin-disorder scattering.

Finally, we treat the problem of asymmetric scattering in the presence of both impurities and phonons. For a one-band model the relaxation tensor becomes $\overleftrightarrow{s} = \overleftrightarrow{s^i} + \overleftrightarrow{s^{ph}}$. However, the matrix element $(s^{ph})_{xy}$ is of odd order (third) in the phonon scattering potential,[9] and therefore its thermal average vanishes except for the higher-order terms, which are very small. Thus Eq. (16) becomes, for one band,

$$Q_s^{is} = -\frac{1}{M_s}\,\frac{\pi^2}{3}\,\frac{k_B^2}{e}\,T\,\frac{d}{d\epsilon_F}\left(\frac{(s^i)_{xy}}{(s^i)_{xx} + (s^{ph})_{xx}}\right). \tag{21}$$

This implies

$$Q_s^{is} \propto T\left[A_1(\rho_i/\rho) + A_2(\rho_i/\rho)^2\right], \tag{22}$$

where A_1 and A_2 are constant coefficients. This contribution is probably important only at low temperatures.

VII. COMBINED PHONON AND SPIN-DISORDER SCATTERING

In order to explain the existence of the constant α in Eq. (2) within the side-jump model, it is necessary to introduce two simultaneous scattering mechanisms, having different temperature dependence and different energy dependence. Since the Kondorskii-Vasileva data mentioned above[4] have been obtained between room temperature and the Curie point, it is natural to assume that these mechanisms are phonon scattering and spin-disorder scattering,[14,15(a)] but not impurity scattering.

Using a one-band model, and writing $s = s_{sp} + s_{ph}$, where ph and sp stand for phonon and spin-disorder, respectively, Eq. (18) becomes, after expanding s_{sp} and s_{ph} around a temperature T_0 and keeping only the linear terms,

$$Q_s^{is} = -T(\alpha + \beta\rho)\,,$$

$$\alpha = -\frac{1}{M_s}\,\frac{\pi^2}{3}\,\frac{k_B^2}{e}\,\frac{\gamma_{Hs}}{\epsilon_F} \times \frac{(r_{sp} - r_{ph})(a_{ph} - a_{sp})\,\rho_{sp}(T_0)\,\rho_{ph}(T_0)}{a_{sp}\rho_{sp}(T_0) + a_{ph}\rho_{ph}(T_0)}\,, \tag{23}$$

$$\beta = -\frac{1}{M_s}\,\frac{\pi^2}{3}\,\frac{k_B^2}{e}\left(\frac{d}{d\epsilon_F}\,\gamma_{Hs} + \frac{\gamma_{Hs}}{\epsilon_F}\,\frac{a_{sp}(r_{sp} - r_n)\,\rho_{sp}(T_0) + a_{ph}(r_{ph} - r_n)\,\rho_{ph}(T_0)}{a_{sp}\rho_{sp}(T_0) + a_{ph}\rho_{ph}(T_0)}\right), \tag{24}$$

where

$$\gamma_{Hs} = \Delta y\, ne^2/\hbar k\,,$$

$$\rho_{sp} = \frac{ms_{sp}}{e^2 n}\,, \qquad \rho_{ph} = \frac{ms_{ph}}{e^2 n}\,,$$

$$a_{sp} = \left(\frac{T_0}{s_{sp}(T_0)}\right)\left(\frac{ds_{sp}}{dT}\right)_{T_0}\,, \qquad a_{ph} = \left(\frac{T_0}{s_{ph}(T_0)}\right)\left(\frac{ds_{ph}}{dT}\right)_{T_0}\,,$$

$$r_{sp} = \left(\frac{\epsilon_F}{s_{sp}}\right)\left(\frac{ds_{sp}}{d\epsilon_F}\right)\,, \qquad r_{ph} = \left(\frac{\epsilon_F}{s_{ph}}\right)\left(\frac{ds_{ph}}{d\epsilon_F}\right)\,,$$

$$r_n = \left(\frac{\epsilon_F}{n}\right)\left(\frac{dn}{d\epsilon_F}\right)\,.$$

The coefficients r_{sp}, r_{ph} are assumed to be independent of T.

Since Eqs. (23) and (24) are based on an expansion around a certain temperature T_0, the temperature range over which they are valid is not necessarily very large, and the coefficients α and β are physically not very meaningful.

In deriving Eqs. (23) and (24) we have also used again our old principle[8] that the value of the side jump Δy should not depend much on the range, strength, or sign of the scattering potential, and we have therefore assumed Δy to have the same value for phonon scattering and for spin-disorder

scattering. According to the first Born approximation this could hold even though spin disorder causes spin-flip scattering, as one can easily show.

We have assumed conduction by one band only (s band). This does not exclude the possibility of s-d transitions induced by the spin disorder, provided the d-band current can be neglected. In fact, this model ensures that the relaxation rate s_{sp} will be well defined.

As in the case of impurity and phonon scattering, the value of the extraordinary Hall conductivity γ_{Hs} is not affected[8] by the nature of the scatterers.

Equations (23) and (24) predict very roughly $Q_s^{is}/T \approx (3\times10^{-10})\ V/T\ \mathrm{K}^2$ for iron at 400 K. This value is within an order of magnitude of the experimental value[4]: $\approx 20\times10^{-10}$. This spin-disorder model seems preferable to the Kondorskii[3] theory, and to our model with combined phonon and impurity presented in Sec. VI, since it leads to $\alpha \neq 0$ even for pure metals.

Note that the Hall conductivity γ_{Hs} appears as a factor in the expression for α in Eq. (23). Thus, any sign change of γ_{Hs} should imply a corresponding sign change for α. This prediction seems to be verified in the Fe-Ni alloy series, where γ_{Hs} changes sign[12(a)] at 85% Ni, while α changes sign[4] at a close-by concentration (70% Ni). The agreement is as good as can be expected in view of the various approximations involved. The sign change of γ_{Hs} is itself caused by the Fermi level moving[15(b)] from the nickel band to the iron band of the alloy.

VIII. OTHER TRANSVERSE EFFECTS

Once the Hall and Nernst coefficients are known, the Righi-Leduc and Ettingshausen coefficients can be calculated, using the Bridgman and Wiedeman-Franz relations.[1,13] The validity of these relations has been investigated on the basis of existing data.[16]

IX. CONCLUSIONS AND FINAL REMARKS

The Hall and Nernst effects of ferromagnets are of special interest, being among the very few transport properties of metals which cannot be treated by semiclassical transport theory.

A fairly transparent and versatile theory of these phenomena has been built based on the concept of side jump.[8] This concept is easy to grasp in space time, but not in the momentum representation. From that point of view, it is very similar to the lifetime of a virtually bound impurity state.

If spin-disorder scattering is also introduced, and if the side jump is assumed to have the same constant value for electron-impurity, electron-phonon, and spin-disorder scattering, then one can derive expressions which agree with existing experimental data for both Hall and Nernst effects [see Eqs. (23) and (24)].

By providing a simple explanation for these large transverse effects, we hope to have answered a question left open since 1879 and 1886, dates when they were observed for the first time[17,18] in ferromagnets.

APPENDIX A: ABSENCE OF ANY ANOMALOUS DRIVING TERM

In this section, we consider the effect of $\vec{E}$ on the scattering of Bloch waves. The field Hamiltonian is $-e\vec{E}\cdot\vec{x} = -e\vec{E}\cdot\vec{R} - e\vec{E}\cdot\vec{q}$, where $\vec{R}$ is the usual Wannier coordinate, and $\vec{q}$ is the transverse electric dipole of a Bloch wave. We assume a periodic crystal potential $U(\vec{x})$, a periodic spin-orbit interaction H_{so}, and a central scattering potential $V(\vec{x})$. The total Hamiltonian is $H = H_p + V(\vec{x}) - e\vec{E}\cdot\vec{R}$, where $H_p = -(\hbar^2/2m)\nabla^2 + U(\vec{x}) + H_{so} - e\vec{E}\cdot\vec{q}$ is the periodic part of H. Note that H_p can be diagonalized completely with Bloch waves ϕ_k satisfying $H_p\phi_k = E_k\phi_k$. To first order in $\vec{E}$, it is sufficient to consider the perturbation by $-e\vec{E}\cdot\vec{q}$ and by $-e\vec{E}\cdot\vec{R}$ separately, and to add the results. We use here a one-band model with carrier charge e which can be positive or negative.

In the presence of $V(\vec{x})$ and of $-e\vec{E}\cdot\vec{q}$ alone, the band is asymmetric,[12(a),12(d)]

$$E_k \approx \hbar^2k^2/2m^* - e\vec{E}\cdot\langle\vec{q}_k\rangle\ , \tag{A1}$$

with $\langle\vec{q}_k\rangle \approx -\frac{1}{2}\vec{k}\times\vec{D}$. Then, to first order in $\vec{E}$, it is sufficient to consider an equilibrium distribution $f^0(E_k)$. The classical current is

$$\vec{j} = \frac{e}{\hbar}\sum_k f^0(E_k)\ \frac{\partial E_k}{\partial\vec{k}}$$

(see Appendix B). But this expression vanishes identically[12(a)] at any time, even for an asymmetric band. There is no acceleration of the electron gas. The situation is similar to that of an impure magnetic metal without space-inversion symmetry, at $\vec{E} = 0$.

In the presence of $-e\vec{E}\cdot\vec{R}$ alone, then consider the following wave functions[12(b)]:

$$\begin{aligned}\phi_K(\vec{x},t) &= u_k(\vec{x})\exp[i(\vec{k}\cdot\vec{x} - \hbar K^2t/2m^* \\ &\qquad + e\vec{E}\cdot\vec{K}t^2/2m^*)]\ , \\ \vec{k} &= \vec{K} + e\vec{E}\,t/\hbar\ , \qquad d\vec{K}/dt = 0\ ,\end{aligned} \tag{A2}$$

where the periodic factor u_k satisfies, as usual,

$$\frac{\hbar^2}{2m}\nabla^2u_k + \frac{2i\hbar^2}{2m}\nabla u_k\cdot\vec{k} - U(\vec{x})u_k - H_{so}u_k + \left(\frac{\hbar^2}{2m^*} - \frac{\hbar^2}{2m}\right)k^2u_k = 0\ , \tag{A3}$$

$$u_k(\vec{x}) = u_k(\vec{x}+\vec{a})\ . \tag{A4}$$

Equations (A2)–(A4) imply, to first order in $\vec{E}$,

$$H_p \phi_K = \frac{\hbar^2}{2m^*}\left(\vec{K}+\frac{e\vec{E}t}{\hbar}\right)^2 \phi_K , \tag{A5}$$

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\phi_K = (H_p - e\vec{E}\cdot\vec{R})\phi_K , \tag{A6}$$

$$\vec{k}\phi_K = \left(\vec{K}+\frac{e\vec{E}t}{\hbar}\right)\phi_K , \tag{A7}$$

where $-e\vec{E}\cdot\vec{q}$ has been neglected in H_p, as explained above. Thus the Bloch waves ϕ_K are solutions[12(b)] of Schrödinger equation [Eq. (A6)] in the presence of $-e\vec{E}\cdot\vec{R}$ [but in the absence of the scattering potential $V(\vec{x})$]. Their wave vector $\vec{k}$ is time dependent. To find a solution in the presence of both $-e\vec{E}\cdot\vec{R}$ and $V(\vec{x})$, we expand

$$\psi = \sum_K c_K(t)\,\phi_K(\vec{x},t) , \tag{A8}$$

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\psi = H\psi . \tag{A9}$$

From Eqs. (A5)–(A9), we obtain

$$-\frac{\hbar}{i}\dot{c}_L = \sum_K V_{LK}\,c_K\,e^{-i(\alpha_K-\alpha_L)} , \tag{A10}$$

where

$$\alpha_K = \hbar K^2 t/2m^* - e\vec{E}\cdot\vec{K}t^2/2m^* ,$$

$$V_{LK} = \iiint d^3x\, u_l^*(\vec{x})\,e^{-i\vec{l}\cdot\vec{x}}\,V(\vec{x})\,u_k(\vec{x})\,e^{i\vec{k}\cdot\vec{x}} ,$$

$$\vec{k} = \vec{K}+e\vec{E}t/\hbar , \quad \vec{l} = \vec{L}+e\vec{E}t/\hbar . \tag{A11}$$

But [9,12(d),12(f)] since $\vec{x} = \vec{R}+\vec{q}$,

$$V(\vec{x}) \approx V(\vec{R}) + \vec{q}\cdot\frac{\partial V}{\partial \vec{R}} , \tag{A12}$$

with

$$\vec{q} \approx -\tfrac{1}{2}\vec{k}\times\vec{D}, \quad \vec{D}\parallel z \parallel \vec{S} .$$

This gives finally, assuming $\vec{K}\parallel x \parallel \vec{E}$, and $\vec{S}\parallel z$, and if the interband elements of $V(\vec{x})$ are neglected:

$$V_{LK} = J_V + iS_z\hbar k_x J^{so}_{LK} , \tag{A13}$$

$$J^V_{LK} = \iiint d^3x\, V(\vec{x})\cos(\vec{K}-\vec{L})\cdot\vec{x} , \tag{A14}$$

$$J^{so}_{LK} = \frac{D}{2\hbar S}\iiint d^3x\,\frac{y}{|\vec{x}|}\left|\frac{\partial V}{\partial \vec{x}}\right|\sin(\vec{K}-\vec{L})\cdot\vec{x} . \tag{A15}$$

Then, to first order in S_z:

$$-\frac{\hbar}{i}\dot{c}_L \approx \sum_K c_K J^V_{LK}\exp\{i\hbar S_z k_x J^{so}_{LK}/J^V_{LK} + i[\alpha_L(t)-\alpha_K(t)]\} . \tag{A16}$$

Assuming the electron to be initially in state K_0, with $K_0\parallel\vec{E}\parallel x$, Eq. (A16) can be integrated in the first Born approximation [$c_{K_0}(t)=1$]:

$$c_L(t) = -\frac{i}{\hbar}J^V_{LK_0}\left(\frac{\pi}{2a}\right)^{1/2}\exp\left(\frac{iS_z(K_0)_x J^{so}_{LK_0}}{J^V_{LK_0}}-\frac{ib^2}{a}\right)\left\{C\left[\left(\frac{2}{a\pi}\right)^{1/2}(at+b)\right] - C\left[\left(\frac{2}{a\pi}\right)^{1/2}b\right] + iS\left[\left(\frac{2}{a\pi}\right)^{1/2}(at+b)\right] - iS\left[\left(\frac{2}{a\pi}\right)^{1/2}b\right]\right\} , \tag{A17}$$

where

$$2b = eE_x S_z\, J^{so}_{LK_0}/J^V_{LK_0} + (\hbar/2m^*)(L^2-K_0^2) ,$$

$$a = -(e/2m^*)(\vec{L}-\vec{K}_0)\cdot\vec{E} ,$$

and C and S are the Fresnel integrals[19]

$$C(x) = \int_0^x \cos\tfrac{1}{2}\pi t^2\, dt; \quad S(x) = \int_0^x \sin\tfrac{1}{2}\pi t^2\, dt .$$

To first order in $\vec{E}$:

$$at+b = \hbar^{-1}[\epsilon_L(t-\Delta t_L) - \epsilon_K(t-\Delta t_L)],$$

where

$$\epsilon_L(t) = (\hbar^2/2m^*)(\vec{L}+e\vec{E}t/\hbar)^2 , \tag{A18}$$

$$\Delta t_L = \frac{m^* S_z J^{so}_{LK_0}}{[L_x-(K_0)_x]J^V_{LK_0}} . \tag{A19}$$

Δt_L is a $\vec{L}$-dependent delay before the scattered wave appears out of the impurity.

Since $C(+\infty)=S(+\infty)=\frac{1}{2}$, $C(-\infty)=S(-\infty)=-\frac{1}{2}$, the C and S functions in Eq. (A17) behave more and more like step functions $H[\epsilon_L(t-\Delta t_L)-\epsilon_K(t-\Delta t_L)]$ when $\vec{E}\to 0$. The step function is defined by $H(y>0)=+\frac{1}{2}$, $H(y<0)=-\frac{1}{2}$, and satisfies

$$H(y) = \int_{-\infty}^{y} dx\,\delta(x) - \tfrac{1}{2} . \tag{A20}$$

The small actual width retained by C and S at $\vec{E}\neq 0$ can be neglected here, since it is independent of $\vec{L}$ direction and has no left-right asymmetry.

If we consider $|c_L(t)|^2$, the same step functions appear there. Using Eq. (A20), we obtain from Eq. (A17):

$$|c_L(t)|^2 = \frac{2\pi}{\hbar}|J^V_{LK_0}|^2\int_0^t dt\,\delta[\epsilon_L(t-\Delta t_L)-\epsilon_K(t-\Delta t_L)] .$$

This implies for the transition probability per unit time $\dot{P}_L$ at time $t+\Delta t_L$:

$$\dot{P}_L(t+\Delta t_L)=\frac{d}{dt}\left|c_L(t+\Delta t_L)\right|^2$$

$$=\frac{2\pi}{\hbar}\left|J^V_{LK_0}\right|^2\delta[\epsilon_L(t)-\epsilon_K(t)]\,. \quad \text{(A21)}$$

This has the usual form for the first Born approximation. The only difference is that, due to the acceleration by $\vec{E}$, electron energies ϵ_L and ϵ_K are time dependent. Also, there is a delay Δt_L, directly related to the existence of the side jump Δy. Since Δt_L is odd with respect to L_y, its effect is indeed to shift the initial location of the center of mass of the scattered wave by a finite amount $\Delta y \approx v_F|\Delta t|$ in the y direction, without affecting its later motion or the scattering rate.

It is interesting that this scattering rate $\dot{P}_L(t+\Delta t_L)$ from state $\vec{k}_0=\vec{K}_0+e\vec{E}t/\hbar$ to state $\vec{l}=\vec{L}+e\vec{E}t/\hbar$ is perfectly symmetric with respect to the plane $(\vec{E},\vec{S})$ in k space, assuming $\vec{k}_0\|\vec{E}\|x$ and $\vec{S}\|z$. This results from $|J^V_{LK0}|$ itself being symmetric.[9] Thus there is no evidence that the influence of $\vec{E}$ on impurity scattering causes any preferential transverse acceleration of the electron, creating subsequently in the periodic lattice a transverse component of the classical current $\vec{j}$.

Therefore, there is no evidence of the existence of an "anomalous driving term" of the general kind proposed by Doniach[12(c)] and by Fivaz,[12(d)] in the first Born approximation.

Central to that conclusion is the fact that we have used the representation of H_p ("physical bands"). This ensures maximum diagonalization of the problem, compatible with Bloch waves of well-defined $\vec{k}$. As a consequence, the off-diagonal part of the density matrix is minimized and can be neglected outside the impurities. Also, the energy eigenvalues E_K are as correct as possible; such is not the case for the work of Doniach [12(c)] or of Fivaz,[12(d)] who work in the representation of $H_p+e\vec{E}\cdot\langle\vec{q}_k\rangle$, not so close to the exact Hamiltonian H, and resulting in eigenvalues ϵ_k.

The mechanisms of Doniach and of Fivaz were themselves proposed as an interpretation of the anomalous driving term found in the Boltzmann equation of Adams and Blount.[12(f)] However, Adams and Blount did not separate out of their statistical distribution f_k of Bloch waves [see their Eqs. (5.9)] the part which actually describes an admixture from excited states, caused by the potential $V(\vec{x})$ and localized in impurities [see our Eqs. (B5) and (B6)]. Such a local admixture to a Bloch wave cannot be represented as a simple Fermi distribution. Thus it seems that the current, which Doniach and Fivaz describe as coming from the acceleration by $\vec{E}$ of a Fermi distribution of Bloch waves in an asymmetric band in the periodic lattice, is actually localized in the impurities and other scattering centers and would be more correctly described by our side-jump model. As mentioned in an earlier paper,[8] the extraordinary Hall resistivity derived from the anomalous driving term is identical to the one derived from the side-jump model, as long as $\omega_c\tau\ll 1$. The side-jump current $\vec{J}$ is $\vec{j}$ dependant rather than $\vec{E}$ dependant, however.

Note that H_p, and $\vec{q}$ itself, are not invariant[9,12(d)] under a gauge transformation. Thus we have to choose a particular gauge[12(d)] in order to write $\vec{q}_k\approx-\frac{1}{2}\vec{k}\times\vec{D}$. But, as long as all calculations are done correctly and completely, all physically measurable quantities, such as Δy, will automatically be given their correct, gauge-invariant value in the end. And, of course, as in electromagnetic theory, the choice of a particular gauge makes for a considerably simpler treatment of our specific, practical problem.

See Appendix B for a complete accounting of currents in a ferromagnet.

APPENDIX B: COMPLETE ACCOUNTING OF CURRENTS IN A FERROMAGNET

Using the same notation as in Appendix A, we calculate the total velocity $\langle\vec{v}\rangle=\langle d\vec{R}/dt\rangle+\langle d\vec{q}/dt\rangle$:

$$\langle d\vec{R}/dt\rangle=\frac{i}{\hbar}\langle[H_p,\ \vec{R}\,]\rangle-\frac{i}{\hbar}\langle[e\vec{E}\cdot\vec{R},\ \vec{R}\,]\rangle$$

$$+\frac{i}{\hbar}\langle[V(\vec{x}),\vec{R}\,]\rangle\,. \quad \text{(B1)}$$

The second term vanishes. The first term is evaluated in the Wannier representation as follows.

Considering Bloch waves ϕ_k satisfying $H_p\phi_k=E_k\phi_k$, we define the Wannier function $W(\vec{x})=\sum_k\phi_k(\vec{x})$ for a given band. Then an arbitrary state ψ of the dilute alloy can be represented by the coefficients c_R, if admixture from other bands is neglected:

$$\psi=\textstyle\sum_R c_R W(\vec{x}-\vec{R})\,. \quad \text{(B2)}$$

We find, after some calculations:

$$\langle W(\vec{x}-\vec{R})|\,(i/\hbar)[H_p,\ \vec{R}\,]\,|W(\vec{x}-\vec{R}\,')\rangle$$

$$=\sum_k\frac{1}{\hbar}\frac{\partial E_k}{\partial\vec{k}}\,e^{i\vec{k}\cdot(\vec{R}-\vec{R}')}=g(\vec{R}-\vec{R}\,')\,, \quad \text{(B3)}$$

where the sum extends over the first Brillouin zone, and where the value of the function g becomes negligible as soon as $|\vec{R}-\vec{R}\,'|$ exceeds one or two lattice cells a. Thus $(i/\hbar)[H_p,\ \vec{R}\,]$ is a fairly local operator in the crystal. Introducing a modified wave function ψ' where the part close to the impurities has been removed

$$\psi'(\vec{x})=\sum_{|\vec{R}|>2a}c_R W(\vec{x}-\vec{R})\,, \quad \text{(B4)}$$

we can write the expectation

$$\langle\psi|\,(i/\hbar)[H_p,\ \vec{R}\,]\,|\psi\rangle=\langle\psi'|\,(i/\hbar)[H_p,\ \vec{R}\,]\,|\psi'\rangle$$

$$+\Delta\langle(i/\hbar)[H_p,\ \vec{R}\,]\rangle\,, \quad \text{(B5)}$$

where

$$\Delta((i/\hbar)[H_p, \vec{R}]) = \sum_{|\vec{R}| \le 2a} \sum_{\vec{R}'} g(\vec{R}-\vec{R}')c_R^* c_{R'} + \sum_{\vec{R}} \sum_{|\vec{R}'| \le 2a} g(\vec{R}-\vec{R}')c_R^* c_{R'} .$$

The first term of Eq. (B5) represents the classical current $\vec{j}$, corresponding to free motion of an electron wave packet in the periodic part of the lattice, while the second term represents motion in the neighborhood of the impurities. Using a Bloch representation for ψ', we write $\psi' = \sum_k a_k \phi_k$, and Eq. (B5) becomes

$$\langle\psi|(i/\hbar)[H_p, \vec{R}]|\psi\rangle = \sum_k |a_k|^2 \frac{\partial E_k}{\partial k}\frac{1}{\hbar} + \Delta((i/\hbar)[H_p, \vec{R}]) . \tag{B6}$$

Using[12(d)] $\vec{q} \approx -\frac{1}{2}\vec{k}\times\vec{D}$:

$$V(\vec{x}) = V(\vec{R}+\vec{q}) \approx V(\vec{R}) + \vec{q}\cdot\frac{\partial V}{\partial \vec{R}} = V(\vec{R}) + H_{so}^{eff} ,$$

where $H_{so}^{eff} = A_{so}^{eff}(\vec{R}\times\vec{k})_z S_z$ is an effective spin-orbit Hamiltonian with a coupling constant A_{so}^{eff} 10^4 times larger than the usual atomic spin-orbit parameter. Thus

$$\frac{i}{\hbar}\langle[V(\vec{x}), \vec{R}]\rangle \approx \frac{i}{\hbar}\langle[H_{so}^{eff}, \vec{R}]\rangle . \tag{B7}$$

We average Eq. (B6) over an ensemble of states ψ, each having probability P_n, and we define $f_k = \sum_n P_n |a_k|^2$.

Writing, moreover, $f_k \approx df_k + f^0(E_k)$, where df_k is the departure from equilibrium, and using the identity

$$\sum_k f^0(E_k)\frac{\partial E_k}{\partial \vec{k}} = 0 ,$$

we obtain from Eqs. (B1), (B2), and (B5)–(B7):

$$\left\langle\frac{d\vec{R}}{dt}\right\rangle = \sum_k df_k \frac{1}{\hbar}\frac{\partial E_k}{\partial \vec{k}} + \Delta\left(\frac{i}{\hbar}[H_p, \vec{R}]\right) + \frac{i}{\hbar}\langle[H_{so}^{eff}, \vec{R}]\rangle . \tag{B8}$$

To first order in $\vec{E}$, the first term may also be written

$$\sum_k df_k \frac{1}{\hbar}\frac{\partial \epsilon_k}{\partial \vec{k}} ,$$

where $\epsilon_k = (\hbar^2/2m^*)k^2$. Thus this classical current $\vec{j}$ is not affected by the existence of asymmetric bands [see Eq. (A1)].

On the other hand, in the stationary state:

$$\left\langle\frac{d\vec{q}}{dt}\right\rangle \approx \frac{1}{2}\vec{D}\times\left\langle\frac{d\vec{k}}{dt}\right\rangle = \frac{1}{2}\vec{D}\times\left(\left\langle\frac{d\vec{k}}{dt}\right\rangle_{field} + \left\langle\frac{d\vec{k}}{dt}\right\rangle_{scat}\right) = 0 . \tag{B9}$$

As a conclusion, the total current $\langle\vec{v}\rangle$ in a ferromagnet is given by Eq. (B8). The first term gives the classical current $\vec{j}$, and is not localized in impurities. It has a transverse component because of the Smit asymmetric scattering[9] on impurities. The general conclusion of Appendix A is that no nonclassical unaccounted transverse effect can influence the coefficients df_k in Eq. (B8). The second and third terms of Eq. (B8) are localized in impurities, where $V(\vec{x}) \neq 0$, and represent the nonclassical side-jump current $\vec{J}$.

It is because of that localization that the calculation of $\vec{J}$ can be reduced to a problem of scattering theory.

Note that, since $[H_p, \vec{R}]$ has no off-diagonal elements in the Bloch representation (except between different bands), only the diagonal part f_k of the density matrix can contribute to the current $\vec{j}$ outside the impurities [Eq. (B8)]. On the other hand, an off-diagonal contribution to $\vec{J}$ exists, and is automatically included in our scattering calculation of $\vec{J}$.

Note also that, when writing $f_k \approx df_k + f^0(E_k)$, we assume f_k to reduce to a simple Fermi distribution $f^0(E_k)$ when $\vec{E} \to 0$. This cannot be strictly true, since f_k refers to an ensemble of alloy functions ψ' which have been made artificially to vanish in the regions of the impurities. The existence of such local "holes" in the ψ' must be reflected in their Fourier spectrum by a broad isotropic contribution $\Delta f(E_k)$, so that actually $f_k = df_k + \Delta f(E_k) + f^0(E_k)$. However, in a dilute alloy this causes only a small error in $\vec{j}$. And this longitudinal, classical, current $\vec{j}$ does not need to be calculated very exactly.

---

[1]T. C. Harman and J. M. Honig, *Thermoelectric and Thermomagnetic Effects and Applications* (McGraw-Hill, New York 1967); H. B. Callen, Phys. Rev. 73, 1349 (1948).

[2]A. W. Smith, Phys. Rev. 33, 295 (1911).

[3]E. I. Kondorskii, Zh. Eksperim. i Teor. Fiz. 45, 511 (1963) [Sov. Phys. JETP 18, 351 (1964)].

[4]E. I. Kondorskii and R. P. Vasileva, Zh. Eksperim. i Teor. Fiz. 45, 401 (1963) [Sov. Phys. JETP 18, 277 (1964)].

[5]For a description of experimental apparatus to correctly measure the isothermal Nernst effect, see A. W. Smith, Phys. Rev. 32, 178 (1911). See also our Ref. 2.

[6]L. E. Gurevich and I. N. Yasievich, Fiz. Tverd. Tela 5, 2620 (1963) [Sov. Phys. Solid State 5, 1914 (1964)]; E. I. Kondorskii, A. V. Cheremushkina, and N. Kurbaniyazov, *ibid.* 6, 539 (1964) [6, 422 (1964)] (see their note added in proof).

[7]S. S. Abelskii, Phys. Met. Metallogr. (USSR) 18, 145 (1964).

[8]L. Berger, Phys. Rev. B 2, 4559 (1970).

[9]J. Smit, Physica 24, 39 (1958).

[10]L. Berger, Phys. Rev. 177, 790 (1969).

[11]K. Meyer, Z. Naturforsch. 10a, 166 (1955).

[12](a) J. Smit, Physica 21, 877 (1955); (b) C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963), p. 193; (c) S. Doniach, in *Optical and Electronic Structure*

of Metals and Alloys, edited by F. Abelès (North-Holland, Amsterdam, 1966), p. 471; (d) R. C. Fivaz, Phys. Rev. 183, 586 (1969); (e) J. M. Luttinger, *ibid.* 112, 739 (1958); (f) E. N. Adams and E. I. Blount, J. Phys. Chem. Solids 10, 286 (1959).

[13]J. M. Ziman, *Electrons and Phonons* (Oxford U. P., Oxford, England, 1960).

[14]R. J. Weiss and A. S. Marotta, J. Phys. Chem. Solids 9, 302 (1959).

[15](a) F. C. Schwerer and L. J. Cuddy, Phys. Rev. B 2, 1575 (1970); (b) E. Ashworth, D. Sengupta, G. Schnakenberg, L. Shapiro, and L. Berger, Phys. Rev. 185, 792 (1969).

[16]D. Rivier, Helv. Phys. Acta 30, 474 (1957); G. Busch, F. Hulliger, and R. Jaggi, *ibid.* 30, 472 (1957); 31, 3 (1958).

[17]E. H. Hall, Phil. Mag. 10, 301 (1880); H. A. Rowland, Am. J. Math. 2, 354 (1879).

[18]A. von Ettingshausen and W. Nernst, Wied. Ann. Physik Chemie 29, 343 (1886).

[19]E. Jahnke and F. Emde, *Tables of Functions* (Dover, New York, 1945).

PHYSICAL REVIEW B VOLUME 5, NUMBER 5 1 MARCH 1972

Low-Temperature Spin Orientation in Cobalt Tutton's Salt. II

Horacio A. Farach and Charles P. Poole, Jr.
Physics Department, University of South Carolina, Columbia, South Carolina 29208
(Received 21 July 1971)

The spin orientation of the Co^{+2} ions in $Co(NH_4)_2(SO_4)_2 \cdot 6H_2O$ calculated in a previous work was extended to include exchange in addition to the dipolar and hyperfine interactions. The exchange was found to have a small effect on the orientation of the spins, but a significant decrease occurred in the value of the minimum energy.

I. INTRODUCTION

Cobalt Tutton's salt $Co(NH_4)_2SO_4 \cdot 6H_2O$ is widely used in attaining low temperatures by adiabatic demagnetization, and therefore there is considerable interest in its properties. Measurements have been made of its crystal structure, specific heat, transition temperature, magnetic susceptibility, g factor, hyperfine coupling constant, and other properties.[1-6] As a result it is desirable to compare these measurements with calculated values. With this aim in mind we computed the ground-state spin orientation of the cobalt ions in cobalt Tutton's salt in a previous work[7] which will be referred to as I. The influence of the dipolar and hyperfine interactions were taken into account explicitly. In the present paper the calculations will be extended to include the effect of exchange.

In an earlier work Garrett[3] had pointed out that four possible interactions should influence the specific heat, namely, (i) the Stark effect, (ii) the dipolar interaction E_{DD}, (iii) the nuclear electronic interaction E_N, and (iv) exchange E_{ex}. Kramers's degeneracy eliminated the need to consider the Stark effect, and in I the dipolar and nuclear electronic interactions were included. Garrett[3] assumed that the relative contributions to the specific heat of the dipolar and nuclear electronic interactions have the following magnitude:

$$|E_{DD}|/|E_N| \sim 1.18, \tag{1}$$

and his reasoning leads one to expect the ratio of interactions (iv) to (iii) to be

$$|E_{ex}|/|E_N| \sim 0.5\,. \tag{2}$$

Our calculations indicate that the relative contributions to the specific heat of these particular interactions are in accordance with the following ratios:

$$|E_{DD}|/|E_N| \sim 1.15\,, \tag{3}$$

$$|E_{ex}|/|E_N| \sim 0.74\,. \tag{4}$$

The method followed in carrying out these calculations will be described after a brief discussion of each of the three relevant interactions. Relation (4) was calculated with $f = 2.5$, as defined in Sec. V; see also Table II.

II. DIPOLE-DIPOLE INTERACTION

Before proceeding with the new calculation it will be convenient to summarize the method adopted in I. The Luttinger-Tisza[8] approach was employed to obtain a dipolar matrix $\underline{a}$ which takes into account the anisotropies[9] of the lattice. It includes the interaction between ions of type A, that between ions of type B, and also the interactions between both types of ions. The 6×6 matrix $\underline{a}$ was diag-