ON THE THEORY OF THE NERNST-ETTINGSHAUSEN EFFECT IN FERROMAGNETIC METALS

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A theory is given of the transverse electric field (the Nernst-Ettingshausen field) which appears in a magnetized ferromagnetic metal when heat flows through it. The theory presented can explain the temperature dependence of the Nernst-Ettingshausen field observed in ferromagnetic metals and the change of sign of the Nernst-Ettingshausen coefficient observed in iron on transition from low to high temperatures. Comparison of the theoretical conclusions with the experimental data shows that nonlocalized electrons make the principal (greater) contribution to the spontaneous magnetization of iron and nickel.

IT is known that the Hall and Nernst-Ettingshausen (NE) effects in isotropic samples of ferromagnetic metals are given by the empirical formulas [1-5]

$$\mathbf{E}_H = (R_0\mathbf{B} + R_s 4\pi\mathbf{I}_s)\times \mathbf{J}, \qquad (1)$$

$$\mathbf{E}_N = -[(Q_0\mathbf{B} + Q_s 4\pi\mathbf{I}_s)\times \nabla T]_{\mathbf{J}=0}, \qquad (2)$$

where $\mathbf{E}_H$ and $\mathbf{E}_N$ are the Hall and NE electric field intensities; R_0 and Q_0 are the field coefficients; R_S and Q_S are the so-called ferromagnetic coefficients of the Hall and NE effects, respectively; $\mathbf{B}$ is the magnetic induction, $\mathbf{I}_S$ is the magnetization, and $\mathbf{J}$ is the electric current density.

The appearance of the magnetization-dependent Hall field component $\mathbf{E}_{HS}$ in ferromagnets is explained by the current theory as the consequence of the spin-orbit interaction between current carriers and lattice ions. [6-8] It has been assumed that the appearance of the NE field component $\mathbf{E}_{NS}$, which also depends on the magnetization, can be explained similarly, but the value of the field $\mathbf{E}_{NS}$ which would be obtained due to the spin-orbit interaction has not yet been calculated. The purpose of the present work is to estimate theoretically the signs, temperature dependence, and order of magnitude of the fields $\mathbf{E}_{NS}$ appearing in ferromagnetic metals due to the spin-orbit interaction between conduction electrons and lattice ions.

1. INTRODUCTION INTO THE DENSITY MATRIX OF TERMS CONTAINING A TEMPERATURE GRADIENT

To calculate the NE field it is necessary to determine the density matrix for a system of electrons disturbed from their equilibrium state by a temperature gradient and an electric field, and to calculate the average electron velocity at right angles to the temperature gradient in the absence of an electric current. We shall first carry out the calculation for the special case when electrons are scattered only on impurities, and then we shall allow for the scattering of electrons on phonons.

A very general method of calculating the transport coefficients, including coefficients of thermal conductivity type, has been given by Kubo et al, [9] who introduced generalized thermal forces into the expression for the density matrix. However, in calculating the transport coefficients it is more convenient to use the approximate solution for the density matrix obtained from the transport equation (see, for example, the work of Andreev and Kosevich [10]). Then the approximate expression, linear in the temperature gradient and magnetization, for the "spontaneous" NE field can be obtained by two equivalent methods: 1) one can solve the approximate equation for the density matrix in the case when the temperature gradient is not equal to zero and then, having calculated the average value of the electron velocity at right angles to the temperature gradient, obtain the required NE field from the condition that the electric current density is zero; 2) one can use the solution of the equation referred to above obtained by Luttinger [6] and Irkhin and Shavrov [8] for the special case when the electron system is acted upon by an electric field and a zero temperature gradient, and then calculate the energy flux at right angles to the electric current. Having thus found the transport coefficient representing the galvanomagnetic Ettingshausen effect (the heat flow at right angles

to the electric current and the magnetization), one can use the Onsager relationship [1] to find the corresponding coefficient for the thermomagnetic NE effect. Both methods give the same result.

We have used the first method because it is simpler.

Let the system considered consist of a fixed number of noninteracting electrons and let it have finite dimensions, with a uniform temperature gradient $\nabla T = \nabla_\alpha T$ so that $x_\alpha \partial T/\partial x \ll T$. Let us consider first the quasiclassical density of the distribution function for this system:

$$\rho_T = \rho_L + f' = Z^{-1} \exp\{\beta(x_\alpha)[\xi(x_\alpha) - \varepsilon_l] N_l\} + f', \quad (3a)$$

where $\beta(x_\alpha) = 1/\kappa T$; ξ and T are, respectively, the chemical potential and the temperature which are functions of the coordinate x_α; ϵ_l and N_l are, respectively, the energy and number of electrons in the state l, characterized by the quasimomentum k, number of the band n and spin $N_l = 0, 1$.

We transform ρ_L in Eq. (3a), representing $T(x_\alpha)$ as a series $T(x_\alpha) = T_0 + x_\alpha \partial T/\partial x_\alpha + \ldots$. Then in the linear approximation with respect to the small parameter $\vartheta = T_0^{-1} x_\alpha \partial T/\partial x$ we obtain

$$\rho_T = Z^{-1} \exp\left\{\beta_0 \left[(\xi_0 - \varepsilon_l) + \frac{\partial T}{\partial x_\alpha} x_\alpha \left(\frac{\partial \xi}{\partial T} - \frac{\xi_0}{T_0} + \frac{\varepsilon_l}{T_0}\right)\right] N_l\right\} + f', \quad (3b)$$

where β_0 is independent of x_α.

Now, following the well-known general method,[9] we define the density operator for the system considered by analogy with Eq. (3b)

$$\hat{\rho}_T = Z^{-1}\{\exp \beta_0 [(\xi_0 \hat{N} - \hat{H}) + \hat{\Delta}_0 + \hat{\Delta}]\} = \hat{\rho}_L + \hat{f}', \quad (4a)$$

where in the linear approximation with respect to the parameter ϑ

$$\hat{\rho}_L = Z_L^{-1} \exp\{\beta_0 [(\xi_0 \hat{N} - \hat{H}) + \hat{\Delta}_0]\} = \hat{\rho} + \hat{f}_0', \quad (4b)$$

$$\hat{\Delta}_0 = \nabla_\alpha T [\partial\zeta/\partial T - \zeta_0/T_0] \hat{x}_\alpha \hat{N} + (\hat{H}\hat{x}_\alpha + \hat{x}_\alpha \hat{H})/2T_0], \quad (4c)$$

$$\hat{\rho} = Z_0^{-1} \exp[\beta_0 (\xi_0 \hat{N} - \hat{H})], \qquad \hat{f}_0' = \hat{\rho} \int_0^{\beta_0} e^{-\lambda \hat{H}} \hat{\Delta}_0 e^{\lambda \hat{H}} \, d\lambda, \quad (4d)$$

and $\mathrm{Sp}(\hat{\rho}\hat{\Delta}) = 0$.

The Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}' + \hat{H}'', \quad (5)$$

where $\hat{H}_0 = \hat{p}^2/2m + U$ contains the periodic potential U with its constant part, $\hat{H}'$ is the nonperiodic (random) potential of the impurities, and $\hat{H}''$ is the part of the Hamiltonian which describes the spin-orbit interaction (cf. formulas (30) and (31) below). $\hat{H}'$ and $\hat{H}''$ are considered to be independent of the time of perturbation, $\hat{N}$ is the electron number operator, and $\hat{x}_\alpha$ is the operator of the electron coordinate x_α. It is easily shown that in the approximation considered here the density matrix ρ_T satisfies the boundary conditions $\beta(x_\alpha) = \kappa^{-1} dS/d\bar{H} = \beta_0 + \kappa \nabla_\alpha T x_\alpha$ (where S is entropy). The operator $\hat{H}$ commutes with $\hat{\rho}$ but does not commute with $\hat{\rho}_L$ since the matrix ρ_L is not the equilibrium density matrix.

Since the operator $\hat{N}$ commutes with $\hat{H}$ and $\hat{\Delta}_0$ there is an obvious equality

$$[\hat{H} - \hat{\Delta}_0, \hat{\rho}_L] = 0. \quad (6a)$$

Moreover, in the approximation linear with respect to the parameter ϑ

$$[\hat{H} - \hat{\Delta}_0, \hat{f}'] = [\hat{H}, \hat{f}']. \quad (6b)$$

From the equation for the density operator $\hat{\rho}_T$, using Eqs. (4a), (4b), (6a), and (6b), we obtain in the same approximation an equation for $\hat{f}'$

$$i(\partial\hat{\rho}_L/\partial t + \partial\hat{f}'/\partial t) = [\hat{H}, \hat{\rho}_L + \hat{f}'] = [\hat{H} + \hat{\Delta}_0, \hat{\rho} + \hat{f}']. \quad (7a)$$

We note that if the system considered is acted upon by an external electric field such that the orders of magnitude of the quantities $eE_\alpha \hat{x}_\alpha$ and $\hat{\Delta}_0$ are equal (cf. the formula (4c)), then in the same approximation the following equation is valid:

$$i(\partial\hat{\rho}_L/\partial t + \partial\hat{f}'/\partial t) = [\hat{H}_T, \hat{\rho} + \hat{f}'], \quad (7b)$$

where

$$\hat{H}_T = \hat{H} - eE_\alpha \hat{x}_\alpha + \hat{\Delta}_0. \quad (5')$$

Let this system be disturbed from equilibrium at $t = -\infty$. For simplicity we shall assume that E_t and $(\nabla_\alpha T)_t$ are parallel to one another and vary with time so that $E_t = Ee^{st}$ and $(\nabla_\alpha T)_t = \nabla_\alpha T e^{st}$. Then $\hat{f}_0'$ and $\hat{f}'$ can be represented in the form $\hat{f}_0' = \hat{f}_0 e^{st}$ and $\hat{f}' = \hat{f} e^{st}$. The equation (7b) for the density matrix reduces then to the form

$$is(\hat{f}_0 + \hat{f}) = [\hat{H}_1 + \hat{H}_2, \hat{\rho}] + [\hat{H}, \hat{f}], \quad (8)$$

where in accordance with Eqs. (5') and (4c)

$$\hat{H}_1 = -[eE_\alpha + (\zeta/T - \partial\zeta/\partial T)\hat{N}\nabla_\alpha T]\hat{x}_\alpha, \quad (9a)$$

$$\hat{H}_2 = \nabla_\alpha T (H\hat{x}_\alpha + \hat{x}_\alpha H)/2T \quad (9b)$$

(here and later we assume that $\hbar = 1$).

In the representation in which the Hamiltonian $\hat{H}_0 + \hat{H}''$ is diagonal we obtain from Eq. (8) the following equations for the matrix elements $\hat{f}$:

[1] Éfros has pointed out to the present author that it is possible to calculate some other transport coefficients of ferromagnetic metals in a similar manner by means of the expression obtained earlier for the Hall coefficient.

$$-isf_{0ll'}+(\varepsilon_l-\varepsilon_{l'}-is)\,f_{ll'}=C_{ll'}+\sum_{l''}(f_{ll''}H_{l''l'}-H_{ll''}f_{l''l'}). \tag{10}$$

Here the indices l combine the indices n and k (n is the number of the band and k is the quasi-momentum); $C_{ll'}$ are the matrix elements of the commutator;

$$\hat{C}=\hat{C}_1+\hat{C}_2=[\hat{\rho},\hat{H}_1]+[\hat{\rho},\hat{H}_2]. \tag{11}$$

The matrix ρ and Eq. (10) include the small parameters $H'_{ll'}$ which makes it possible to expand $C_{ll'}$ into a series of powers of these parameters beginning from the zero-order term, and to solve successively the family of equations obtained from Eq. (10). Below we shall denote the order of the terms of expansion of the various quantities with respect to the parameter $H_{ll'}$ by a superscript in parentheses.

In solving Eq. (10) we shall follow the method described by Kohn and Luttinger,[11] who considered the case when $\nabla T = 0$. If, following this method, we leave first in Eq. (10) the terms of the first order and calculate the nondiagonal matrix element $\hat{f}^{(-1)}_{ll'}$ and then substitute it into Eq. (10) with terms of the zero order, we find that for $\epsilon_l = \epsilon_{l'}$ and $s \to 0$ this equation goes over the usual Boltzmann transport (kinetic) equation. In fact, using Eqs. (9) and (11), we find:

$$C^{(0)}_l=i\left[eE_\alpha+\left(\frac{\zeta}{T}-\frac{\partial\zeta}{\partial T}\right)\nabla_\alpha T-\frac{\varepsilon_l}{T}\nabla_\alpha T\right]\frac{\partial\rho_l}{\partial k_\alpha}. \tag{12}$$

Substituting $f^{(-1)}_l$ and $C^{(0)}_l$ into Eq. (10), assuming $\epsilon_l = \epsilon_{l'}$, rejecting the terms higher than the zeroth order and proceeding to the limit $s = 0$, we obtain

$$F^l_\alpha\frac{\partial\rho_l}{\partial\varepsilon_l}v^l_\alpha+2\pi\sum_{l'}|H'_{ll'}|^2\delta(\varepsilon_l-\varepsilon_{l'})(f^{(-2)}_l-f^{(-2)}_{l'})=0 \tag{13}$$

$$F^l_\alpha=eE_\alpha-\left(\frac{\varepsilon_l-\zeta}{T}+\frac{\partial\zeta}{\partial T}\right)\nabla_\alpha T, \tag{14}$$

which is identical with the usual transport equation for the case of scattering of electrons on impurities. Thus our selection of the density operator leads, in the zeroth approximation with respect to $H'_{ll'}$, to the same results as the quasiclassical theory.

The average electron velocity $\bar{v}_\beta$ in the direction at right angles to $\nabla_\alpha T$ is

$$\bar{v}_\beta=\bar{v}_{\beta1}+\bar{v}_{\beta2},$$

$$\bar{v}_{\beta_1}=\sum_l(f_{0l}+f_l)\,v^l_\beta,\qquad \bar{v}_{\beta2}=\sum_{l\neq l'}(f_{0ll'}+f_{ll'})\,v^{l'l}_\beta, \tag{15}$$

where $v^{ll'}_\beta = i[\hat{H},\hat{x}_\beta]^{ll'}$ are the matrix elements of the velocity.

The spin-orbit interaction does not give any first-approximation corrections to the energy ϵ_l and to $|H'_{ll'}|^2$ and therefore it does not affect v^l_β and ρ_l; consequently it does not alter $f^{(-2)}_l$ calculated in solving Eq. (13). This means that $\bar{v}^{(-2)}_\beta = 0$. Thus we cannot calculate the anomalous Hall and NE fields by means of the usual zeroth-order transport equation.

In calculating $\bar{v}_\beta$ we restrict ourselves to calculating the terms $\bar{v}^{(-1)}_\beta$ and $\bar{v}^{(0)}_\beta$. Equation (10) differs essentially from the corresponding equation for the special case, when $\nabla T = 0$, only in that it contains the commutator C_2 which, as well as the operator $\hat{x}_\alpha$, also includes the operator $\hat{H}$. The commutator C_1 differs from the commutator C, which occurs in the equation for the special case only by the factor in front of $\hat{x}_\alpha$. Thus to obtain the equations for $f^{(-1)}_l$ and $f^{(0)}_l$ and to calculate $f^{(0)}_{ll'}$ from Eq. (10) we can use the known[6,11] expressions for C. In addition we must find the expressions for $(C_2)^{(0)}_{ll'}$, $(C_2)^{(1)}_l$, $(C_2)^{(1)}_{ll'}$ and $(C_2)^{(2)}_l$.

In the representation in which the Hamiltonian $\hat{H}_0 + \hat{H}''$ is diagonal the matrix elements of the operator x_α are equal to

$$x^{ll'}_\alpha=i\left(\frac{\partial}{\partial k_\alpha}\delta_{ll'}+J^{ll'}_\alpha\delta_{kk'}\right), \tag{16}$$

where $J^{ll'}_\alpha$ are the functions introduced in[12]:

$$J^{ll'}_\alpha=\int w^*_{nk}\frac{\partial}{\partial k_\alpha}w_{n'k}\,d^3x_\alpha, \tag{17}$$

and w_{nk} are periodic functions of the coordinates which occur in the Bloch wave function $\psi_l = \exp(ik_\alpha x_\alpha)w_{nk}$. Using Eqs. (11), (9b), (16) and (4d), we obtain

$$(C_2)^{(0)}_{ll'}=\frac{1}{2}\,iT_0^{-1}\nabla_\alpha T\,(\rho_l-\rho_{l'})\,(\varepsilon_l+\varepsilon_{l'})\,J^{ll'}_\alpha\,\delta_{kk'}. \tag{18}$$

In calculating $C_{ll'}$ we make the same assumption as Luttinger[6] as regards $\hat{H}'$, from which, in particular, it follows that the matrix elements $H'_{ll'}$ vanish when $k = k'$, i.e.,

$$H'_{ll'}\delta_{kk'}=0. \tag{19}$$

The matrix elements $(C_2)_l$ and $(C_2)_{ll'}$, like the matrix elements C_l and $C_{ll'}$ in the case when $\nabla T = 0$, occur in the equations for $f^{(-1)}_l$ and $f^{(0)}_l$. in the form of sums of the following type in which the indices $(n - k) \geq 0$:

$$(\Sigma_2)^{(n)}_0=\lim_{s\to0}(\Sigma_2)^{(n)};$$

$$\left(\sum\nolimits_2\right)^{(n)}=(C_2)^{(n)}_l+\sum_{l'}\left[\frac{(C_2)^{(n-1)}_{ll'}H'_{ll'}}{\omega_{ll'}-is}-\frac{H'_{l'l}(C_2)^{(n-1)}_{ll'}}{\omega_{l'l}-is}\right]$$

$$+\sum_{l'l''}\left[\frac{(C_2)^{(n-2)}_{ll'}H'_{l'l''}H'_{l''l}}{(\omega_{ll'}-is)(\omega_{l''l'}-is)}-\frac{H'_{ll''}(C_2)^{(n-2)}_{l''l'}H'_{l'l}}{(\omega_{ll'}-is)(\omega_{l''l}-is)}\right]+\text{c.c.}; \tag{20}$$

here $\omega_{ll'} = \epsilon_l - \epsilon_{l'}$

Using Eq. (19) and substituting Eq. (18) into Eq. (20) we find $(\Sigma_2)^{(1)} = 0$. Hence it follows that neither the matrix elements C_2 nor the elements C_1 occur in the transport equation with first-order terms. Consequently in the case considered this equation has the same form as in the special case, when $\nabla T = 0$, with the difference that now in place of eE_α it has everywhere F_α^l (cf. Eq. (14)).

Separating out in the transport equation the second-order terms containing first-approximation corrections, linear in spin, due to the spin-orbit interaction, we obtain an equation for the correction to $f_l^{(0)}$ due to this interaction. In order to derive such an equation for the general case it is of course necessary to replace the matrix elements $C_{ll'}$ by $(C_1)_{ll'}$ in a similar equation for the special case, when $\nabla T = 0$ (cf. Eq. (11)), and to include in this equation the terms of the sum $(\Sigma_2)_0^{(2)}$ containing the corrections due to the spin-orbit interaction referred to above. Moreover, it is necessary to replace eE_α with F_α^l in the expressions for $f_l^{(-1)}$ and $f_l^{(0)}$ which occur in this equation.

The equation obtained in this way, like the corresponding equations for the special case when $\nabla T = 0$ (cf. Eqs. (2.50), (2.47) and (2.6) in [6] and Eq. (19) in [8]), is quite complex. It may be simplified by neglecting the terms containing the nondiagonal matrix elements $J^{ll'}\delta_{kk'}$, i.e., the terms which are due to allowing for the interband transitions. The solution of such an approximate transport equation for $f_l^{(0)}$ has the following form:

$$f_l^{(0)} = F_\alpha^l (\varphi_\alpha^l)^{(0)}, \qquad (21)$$

where the quantity $(\varphi_\alpha^l)^{(0)}$ is identical with the multiplier of eE_α in the special solution when $\nabla T = 0$.

Up to now we have considered the case when the electrons are scattered on impurities. However, we can show similarly that in the case when the electrons are scattered only on phonons the solution of the corresponding approximate transport equation for $f_l^{(0)}$ also leads to Eq. (21). Moreover, if we restrict ourselves to the case when the temperature T is higher than the Debye temperature Θ_D, we can obtain an expression for $f_l^{(-1)}$ when $\nabla T \neq 0$ with allowance for the scattering of electrons on both phonons and impurities.

The calculation of $f_l^{(-1)}$ in the general case when electrons are scattered on impurities and phonons and when $\nabla T \neq 0$ was carried out by the author of the present paper together with Abdurakhmanov. The following formula was then obtained for $f_l^{(-1)}$:

$$f_l^{(-1)} = -iF_\alpha^l \frac{\partial \rho_l}{\partial \varepsilon_l} \frac{\tau_l}{\tau_{0l}} \frac{\varepsilon_F}{3\nu|\bar{\varphi}|} \sum_{\mu=\beta,\gamma} \left(\frac{\partial J_\alpha^l}{\partial k_\mu} - \frac{\partial J_\mu^l}{\partial k_\alpha} \right) k_\mu, \qquad (22)$$

where $\tau_l^{-1} = \tau_{0l}^{-1} + \tau_{pl}^{-1}$; τ_{0l} and τ_{pl} are the relaxation times for the scattering of electrons on impurities and phonons respectively; ϵ_F, ν and $|\bar{\varphi}|$ are the Fermi energy, the number of scattering impurity centers per unit volume, and the average absolute value of the scattering impurity potential, respectively.

We shall now derive formulas for $\bar{v}_\beta^{(-1)}$ and $\bar{v}_\beta^{(0)}$ for the case when $\nabla T \neq 0$. Substituting Eq. (22) in Eq. (15) we find

$$\bar{v}_\beta^{(-1)} = i \frac{\varepsilon_F}{3\nu|\bar{\varphi}|} \sum_l F_\alpha^l \frac{\partial \rho_l}{\partial \varepsilon_l} \frac{\tau_l}{\tau_{0l}} \left(\frac{\partial J_\beta^l}{\partial k_\alpha} - \frac{\partial J_\alpha^l}{\partial k_\beta} \right) k_\beta v_\beta^l. \qquad (23)$$

From Eq. (23) it follows that in the general case $\bar{v}_\beta^{(-1)}$ is inversely proportional to the total electrical resistance ρ_0 and not to the residual resistance.

We shall calculate $\bar{v}_\beta^{(0)}$ for the case when the electrons are scattered on phonons. The additional term in $\bar{v}_\beta^{(0)}$ obtained on allowing for the scattering of electrons on impurities contains, like $\bar{v}_\beta^{(-1)}$ [cf. Eq. (23)], the multiplier τ_l/τ_{0l} and is found to be one or two orders of magnitude smaller than the principal term when $T > \Theta_D$. The formula for $(\bar{f}_l^{(0)})_{\nabla T=0}$ in the case which is of interest to us was obtained by Irkhin and Shavrov [cf. Eq. (21) in [8]]. Substituting into Eq. (21) the quantity φ_α^l found from this formula [2], we obtain

$$f_l^{(0)} = -iF_\alpha^l J_\alpha^l \partial \rho_l / \partial \varepsilon_l. \qquad (24)$$

Substituting $f_l^{(0)}$ and f_{0l} from Eq. (4c) [3] into Eq. (15), we find

$$\bar{v}_{\beta 1}^{(0)} = -ieE_\alpha \sum_l \frac{\partial \rho_l}{\partial \varepsilon_l} J_\alpha^l v_\beta^l. \qquad (25)$$

We must find now the "nondiagonal" part of $\bar{v}_{\beta 2}^{(0)}$ of the average velocity. Using Eq. (16) we obtain the nondiagonal matrix elements of the velocity:

$$v_\beta^{ll'} = -\omega_{ll'} J_\beta^{ll'} \delta_{kk'}. \qquad (26)$$

Since the matrix element $f_{ll'}^{(-1)}$ contains the multiplier $H_{ll'}^{(1)}$, the quantity $\bar{v}^{(-1)}$ vanishes on the strength of Eq. (19). For the same reason the terms containing $f_{ll'}^{(-1)}$ vanish from the expression for $\bar{v}_{\beta 2}^{(0)}$. Consequently, we obtain for $\bar{v}_{\beta 2}^{(0)}$ the following formula, which is similar to the formula in the case when $\nabla T = 0$, but with the addition of a sum containing matrix elements of the commutator C_2 and the term with $f_{0ll'}$:

$$\bar{v}_{\beta 2}^{(0)} = \sum_{l,\,l'} [(C_1 + C_2)^{(0)} J_\beta^{ll'} - f_{0ll'} \omega_{l'l} J_\beta^{l'l}] \delta_{k'k}. \qquad (27)$$

[2] It should be remembered that in the work of Irkhin and Shavrov[8] the quantity e represents the absolute value of the electronic charge.

[3] The quantities f_{0l} and $f_{0ll'}$ are calculated by means of Feynman's theorem.

Substituting here C_1, C_2 and $f_{0ll'}$ and using Eqs. (11), (9), (14), and (19) we obtain

$$\bar{v}^{(0)}_{\beta 2} = ieE_\alpha \sum_{l,l'} \rho_l (J^{ll'}_\beta J^{l'l}_\alpha - J^{ll'}_\alpha J^{l'l}_\beta) = ieE_\alpha \Sigma \rho_l \left(\frac{\partial J^l_\beta}{\partial k_\alpha} - \frac{\partial J^l_\alpha}{\partial k_\beta} \right)$$

$$= - ieE_\alpha \sum_l \frac{\partial \rho_l}{\partial \varepsilon_l} (J^l_\beta v^l_\alpha - J^l_\alpha v^l_\beta). \quad (28)$$

Combining Eqs. (28) and (25), we find

$$\bar{v}^{(0)}_\beta = - ieE_\alpha \sum_l \frac{\partial \rho_l}{\partial \varepsilon_l} J^l_\beta v^l_\alpha, \quad (29)$$

i.e. $\bar{v}^{(0)}_\beta$ does not depend explicitly on the temperature gradient (the expression for $\bar{v}^{(0)}_\beta$ is the same as in the case when $\nabla T = 0$).

Having determined J^l_β we can calculate the NE field at temperatures above the Debye temperature by means of Eqs. (23) and (29).

2. INTRODUCTION OF A TERM DEPENDING ON THE AVERAGE MAGNETIC MOMENT OF ELECTRONS BOUND TO IONS INTO THE SPIN-ORBIT INTERACTION OPERATOR

An expression for J^l_β was obtained by Karplus and Luttinger [12] and by Irkhin and Shavrov.[8] However, they took into account only that part of the spin-orbit interaction energy which is related to the average magnetic moment of conduction electrons contributing to the spontaneous Hall effect. This is equivalent to the assumption that the localized electrons, i.e., those bound to ions, make no contribution to the average magnetic moment of ferromagnetic metals. Such an assumption is known to be wrong for rare-earth metals, in which the principal contribution to I_S comes from the f-shell electrons, and the correctness of the assumption is not obvious for the iron group metals. Consequently, in calculating J^l_β it is necessary to allow for the interaction of the spin of localized electrons, i.e., those bound to ions, with the conduction electron orbits.[4)] There are various ways of introducing terms describing this interaction into the operator $\hat{H}''$; in particular, one can use the semiclassical model, employed by Heisenberg [13] in introducing the spin-orbit interaction operator for a system of two electrons, or one can employ the more rigorous method proposed in the work of Gaunt and Oppenheimer.[14]

The energy H''_e of a dipole with moment $\mathbf{M}_e$, momentum p and coordinates x, y, z in an electric field with a potential V(x, y, z), produced, for example, by fixed identical point charges q, is known to be

$$H''_e = (mc)^{-1} [\nabla V \ \mathbf{p}] \mathbf{M}_e = - (2m^2c^2)^{-1} [\nabla U \ \mathbf{p}] \mathbf{M}_e/\mu_B,$$

where U = eV is the potential electric energy which an electron would have when superimposed on a dipole. If we place identical magnetic dipoles with moments $\mathbf{M}_i$ at the points occupied by the identical charges q producing the electric field with potential V, the total energy of the dipoles H''_i in the magnetic field produced by a particle with a charge $-q'$, momentum p and coordinates x, y, and z, is given by

$$H''_i = - (mc)^{-1} [\nabla V' \ \mathbf{p}] \mathbf{M}_i = (2m^2c^2)^{-1} [\nabla U \ \mathbf{p}] \sigma_0 \mathbf{M}_i/\mu_B,$$

where U = eV is the potential electric energy which an electron would have at the site occupied by a particle $\sigma_0 = q'/q$.

Thus, the energy of a classical electron with a magnetic moment $\mathbf{M}_e$ moving in a lattice of ions with magnetic moments $\mathbf{M}_i$ and charges $|e|/\sigma_0$ localized near the centers of the ions, is given by

$$H'' = - (2m^2c^2)^{-1} [\nabla U \ \mathbf{p}] (\mathbf{M}_e - \sigma_0 \mathbf{M}_i)/\mu_B. \quad (30)$$

Introducing into the above formula the momentum operator in place of p and adjusting the numerical multiplier so that for $\mathbf{M}_i = 0$ the operator $\hat{H}''$ is identical with the spin-orbit interaction operator for one electron, we obtain the required expression for $\hat{H}''$ with terms allowing for the interaction of the spins of the electrons bound to ions with the conduction electron orbits, i.e.,

$$\hat{H}'' = - (4m^2c^2)^{-1} [\nabla U \ \hat{\mathbf{p}}] (\mathbf{M}_e - \sigma_0 \mathbf{M}_i)/\mu_B. \quad (31)$$

We have assumed above that the densities of the magnetic moment and charge of the localized electrons are concentrated at the nuclei. This assumption is approximately true only for rare-earth metal ions. In the case of transition metals the densities of the magnetic moment and charge are smeared out and therefore the formula for $\hat{H}''$ should be written thus:

$$\hat{H}'' = - (4m^2c^2)^{-1} \{ [\nabla U_0 \hat{\mathbf{p}}] \mathbf{M}_e - [\nabla U_1 \hat{\mathbf{p}}] \ \mathbf{M}_i \}. \quad (31')$$

where

$$U_0 = e \int \frac{\rho \, d\Omega'}{|R - R'|}, \qquad U_1 = \frac{e^2}{M_i} \int \frac{\mu \, d\Omega'}{|R - R'|}; \quad (C)$$

ρ and μ are, respectively, the charge and magnetic

[4)] The division of electrons into localized and nonlocalized is arbitrary. All electrons of the outer shells participate to some extent in conduction in a metal but the average velocities in the direction of the electric field and the average magnetic moments of electrons belonging to different bands are different. In the one-electron theory this difference may be allowed for by a model which considers nonlocalized and "localized" electrons. Then the average charge and magnetic moment densities of the nonlocalized electron are higher near lattice ions.

moment densities of the bound electrons and nuclei.

Using this more general formula and carrying out calculations similar to those of Irkhin and Shavrov[8] and Karplus and Luttinger,[12] we obtain the following expression for J_β^l:

$$J_\beta^l = \frac{i\pi\rho_0^l\,[\mathbf{k}\Delta\mathbf{M}]_\beta}{3m^2c^2\mu_B\, m^*\omega_{nn'}^2}, \tag{32}$$

where

$$\Delta\mathbf{M} = \mathbf{M}_e - \sigma\mathbf{M}_i, \quad \sigma = \rho_0^l/\rho_1^l \approx \sigma_0, \tag{D}$$

$$\rho_j^l = \frac{1}{4\pi}\int w_{nk}^*\,(\nabla^2 U_j)\,w_{nk}\,d^3x_\alpha \quad (j=0,1). \tag{33}$$

From Eq. (32) it is clear that the sign of iJ_β^l and consequently the sign of $\bar{v}_\beta$ and the signs of the coefficients R_S and Q_S depend on the sign of ΔM_γ, i.e., on the mutual orientation and magnitudes of $\mathbf{M}_e$ and $\mathbf{M}_i$.

3. CALCULATION OF THE E_{Ns} COMPONENT OF THE NERNST-ETTINGSHAUSEN FIELD

The field E_N for the isothermal Nernst-Ettingshausen effect is

$$(E_N)_\beta = -n_0 e\bar{v}_{N\beta}\rho, \tag{34}$$

where $\bar{v}_{N\beta}$ represents the value of $\bar{v}_\beta$ obtained for zero density of the electric current j_α; ρ is the electrical resistivity; n_0 is the number of carriers. To calculate $\bar{v}_{N\beta}$ it is necessary to determine the intensity of the field $(E_N)_\alpha$ from the condition that the current density along the α-axis is zero and to substitute the values of F_α^l corresponding to this field intensity into Eqs. (23) and (29).

We shall use for $(E_N)_\alpha$ an expression obtained in the effective-mass approximation, i.e.

$$(E_N)_\alpha = -\frac{n_0\pi^2\varkappa^2 T}{3|e|\varepsilon_F}\left(r+\frac{1}{2}\right)f_1\nabla_\alpha T; \tag{35}$$

$$f_1 = \langle\tau_F/m^*\rangle/\langle\tau_F/|m^*|\rangle, \tag{36}$$

where τ_F is the value of the relaxation time τ_l when $\epsilon_l = \epsilon_F$; $\langle\tau_F/m^*\rangle$ is the average value of τ_F/m^* over all the conduction bands and r is a positive or negative parameter depending on the nature of the scattering processes. For the quadratic dispersion law the value of r is found from the relationship $\tau_l = \tau_0\epsilon_l^{r-1/2}$, where τ_0 is independent of ϵ_l. For the case of strong degeneracy in metals at temperatures at which the electrical resistance is mainly due to scattering on phonons, r = 2. It is clear from Eq. (35) that for n-type conduction, when $f_1 > 0$, $(E_N)_\alpha$ is directed against the temperature gradient but for p-type conduction, when $f_1 < 0$, it is directed along that gradient.

We shall select the coordinate axes so that the x-axis is directed opposite to the temperature gradient and the z-axis lies along the magnetization. Then, using Eqs. (35), (14), (23), (29), and (34), after integrating with respect to k, summing over n, and rejecting terms containing $\kappa T/\epsilon_F$ in the third degree or higher, we obtain

$$(E_{Ns})_y = E_{Ns}^{(-1)} + E_{Ns}^{(0)} = 4\pi I_s(\alpha+\beta\rho)\,T\frac{\partial T}{\partial x}, \tag{37}$$

where

$$\alpha = \frac{2an_0(r+1/2)}{3\nu|\bar{\varphi}|}(1-f_1f_2)\,\rho_{res}, \tag{38}$$

$$\beta = \frac{an_0(r+1/2)}{\varepsilon_F}f_1f_3, \tag{39}$$

$$a = \frac{\pi^2\varkappa^2|e|\langle\rho_0^l/|m^*|\rangle}{36\,m^2c^2\mu_B\langle\omega_{nn'}^2\rangle I_s}\Delta M_z, \tag{40}$$

$$f_2 = \frac{\langle\tau_F\rho_0^l/m^*\rangle}{\langle\tau_F\rho_0^l/|m^*|\rangle}, \qquad f_3 = \frac{\langle\rho_0^l/m^*\rangle}{\langle\rho_0^l/|m^*|\rangle} \tag{41}$$

and ρ_0^l is determined from Eq. (32).

From Eqs. (37)—(41) and (2) it follows that the NE coefficient Q_S, corresponding to the NE field component considered here, is related to T and the electrical resistivity ρ by a simple relationship:

$$Q_s = -(\alpha+\beta\rho)\,T. \tag{42}$$

In the case where the carriers are of one type only, $f_1f_2 = f_1f_3 = 1$ and it follows from Eqs. (38), (39) and (42) that

$$Q_s = -an_0(r+1/2)\,\rho T/\varepsilon_F. \tag{43}$$

From Eqs. (43) and (40) it follows that $Q_S < 0$ for $\Delta M_Z > 0$, when the nonlocalized electrons make the principal contribution to the spontaneous magnetization (because $r > -1/2$ in metals). The same equations lead to the conclusion that $Q_S > 0$ for $\Delta M_Z < 0$. As shown below, this contradicts the conclusions which may be made from the experimental data for iron, nickel, cobalt, and their alloys. Hence it follows that for these metals and alloys it is not permissible to restrict oneself to one type of carriers in the calculation of the NE effect.

From Eqs. (38), (40), and (41) it is clear that in metals the sign of α is the same as ΔM_Z (because f_1f_2 is always smaller than unity and $r \approx 2 > -1/2$). Thus, from the experimental data on the sign of α we can tell whether localized or nonlocalized electrons make the main contribution to the spontaneous magnetization.

From the work of Ivanova[5], the present author

and Vasil'eva [15] on the temperature dependence of Q_S for iron, and nickel and their alloys, it is evident that Eq. (42) describes well the dependence of Q_S on T and that $\alpha = 0$ for iron and nickel. Thus, from the theoretical formulas (38), (40), and (41) and from the experimental data it is clear that the spontaneous magnetization of iron and nickel is mainly due to the magnetic moments of nonlocalized electrons.

The parameter a can easily be related to the Hall coefficient R_S. It follows from Eqs. (29), (32), (40) and (41) that the spontaneous Hall field[5)] is

$$(E_{Ns})_y = -n_0 e \rho (v_y)_{\nabla T=0} = -an_0 |e| f_3 \rho E_x 4\pi I_s. \quad (44)$$

Comparing Eqs. (44) and (1) we find

$$R_s \rho^{-2} = -an_0 |e| f_3. \quad (45)$$

For the special case $M_i = 0$ Eq. (45) gives the formula for R_S deduced by Irkhin and Shavrov.[8] Using Eqs. (39)—(41) and (45) we can estimate the order of magnitude of the quantity β by substituting into these equations the values of $R_S\rho^{-2}$ known from experiment. Comparison of the values of β calculated in this way with the observed ones shows that the theory proposed here gives the correct order of magnitude for the Nernst-Ettingshausen field.

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[5)] The Hall field component related to $\bar{v}_\beta^{(1)}$ is small; this may be explained by the smallness of the quantity f_2. On the other hand, as shown above, the NE field component related to $\bar{v}_\beta^{(-1)}$ is by no means small [cf. Eqs. (38) and (39)].

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