$c+eb\rho$ varies by about $\pm 3\%$ from its average value over the complete experimental range. For small values of the reaction order, n, it can be stated that for experiments considered in this work, a defect concentration reaction of the type of Eq. (3) will result in a variation of resistivity which obeys Eq. (4).

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Theory of the Hall Effect in Ferromagnetic Substances

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The Hall effect in ferromagnetic substances is computed on the basis of a simple model, making use of the transport theory of Kohn and Luttinger. The calculation is rigorous, but assumes a slowly varying scattering potential, a simple band, and very few conduction electrons. None of these assumptions are very realistic for a true ferromagnet, but we are interested here in only giving a discussion of the types of contributions which can occur. Terms related to those previously found by Smit and by Karplus and Luttinger, and some new ones, are found. In addition, some comments of Smit on the general problem of the ferromagnetic Hall effect are discussed.

1. INTRODUCTION

IN recent years there has been considerable discussion of the anomalous Hall effect in ferromagnetic substances, from several points of view. All serious attempts to explain this phenomenon have used as a basic model magnetically polarized electrons moving under the influence of an external field, and have attributed its origin to the presence of spin-orbit coupling. The difference has been in the effect of the spin-orbit coupling considered. Karplus and Luttinger looked for contributions which arise from a modification of the acceleration effects due to the electric field, and from off-diagonal parts of the density matrix. Smit, on the other hand, considered the modification which occurs in the scattering processes within the framework of conventional transport theory. Both of these theories give results which are not in contradiction with experiment, though neither of them fits all the data. On the other hand, some of the conclusions of the theory of Karplus and Luttinger have been seriously questioned by Smit, so that the entire subject has recently been shrouded in a thick fog.

For this reason, we thought it worth while to consider the subject anew, from a somewhat different point of view. There exists a model (for impurity-limited resistivity) in which the entire transport theory can be put on a rigorous and systematic basis. This is the theory of Kohn and Luttinger,[1] which develops the stationary-state density matrix of the system in powers of the strength of the scattering potential. Using this model, we have calculated the entire anomalous Hall effect. Terms of the Smit type, the Karplus-Luttinger type, and some others, all appear automatically in this treatment. Although the model itself is not very realistic, and the further simplification necessary to complete the calculation makes it even less so, we still believe it is of some interest in showing the types of contributions which can occur.

The paper is organized as follows. In Sec. 2 the theory of KLI is summarized and reduced to a usable form without any further approximations. In Sec. 3, the contribution of the spin-orbit coupling (which gives rise to the Hall current) is separated out. In Sec. 4 the equations are solved, and the Hall current is calculated rigorously in the effective-mass limit. In Sec. 5 we discuss the results and compare them with the previous ones. Finally, in Appendix A, some of the criticisms of Smit are considered within the framework of the present theory.

2. GENERAL THEORY

In this section we shall develop the general formulas which enable us to calculate the contribution of spin-orbit coupling to the Hall effect. From KLI, we can expand that part of the density matrix which is linear in the external field (f), in ascending powers of λ (which is some dimensionless measure of the strength of the scattering potential). The leading term in f is of order λ^{-2}, and to this order conventional transport theory holds. The new features of KLI (corrections to transport equation, contributions from off-diagonal ele-

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[1] W. Kohn and J. M. Luttinger, Phys. Rev. **108**, 590 (1957). We shall refer to this paper as KLI in what follows. As in KLI, we shall not indicate explicitly here the vector character of k or r. Thus $e^{ik\cdot r}$ means $e^{i\mathbf{k}\cdot\mathbf{r}}$ and $k\neq k'$ means $\mathbf{k}\neq\mathbf{k}'$ throughout.

ments of f) arise only if we go two orders further in λ, i.e., to λ^0. In the "l representation" [that is, the representation of Bloch waves for the unperturbed Hamiltonian, l standing for the index pair (n,k)] the density matrix f may be written as follows. The off-diagonal terms $f_{ll'}(l\neq l')$ are given by [KLI, Eq. (116), (117), (118)]

$$f_{ll'}=f_{ll'}{}^{(-1)}+f_{ll'}{}^{(0)}, \tag{2.1}$$

where

$$f_{ll'}{}^{(-1)}=\frac{1}{d_{ll'}{}^{-}}(f_l-f_{l'})H_{ll'}, \tag{2.2}$$

and

$$f_{ll'}{}^{(0)}=\frac{1}{d_{ll'}{}^{-}}\times\left[C_{ll'}{}^{(0)}+\sum_{l''}{}'H_{ll''}H_{l''l'}\left(\frac{f_l-f_{l''}}{d_{ll''}{}^{-}}-\frac{f_{l''}-f_{l'}}{d_{l''l'}{}^{-}}\right)\right]. \tag{2.3}$$

The notation is the following: $f_l\equiv f_{ll}$, the diagonal elements of the density matrix. $d_{ll'}{}^{\pm}\equiv\omega_{ll'}\pm is$, where $\omega_{ll'}$ is the difference in energy between the two Bloch states l and l', and s is an infinitesimal positive number. $H_{ll'}$ are the matrix elements of the scattering potential. The notation $\sum'$ means that *all* index equalities should be excluded from the summation, which means for (2.3) that $l''\neq l$ or l'. Finally, the matrix elements $C_{ll'}$ are the matrix elements of the "commutator" $C\equiv -eE_\alpha(\rho,x_\alpha)$, ρ being the equilibrium density matrix in the presence of the scattering centers. $C_{ll'}{}^{(0)}$ are the terms of order λ^0 in this matrix element, $C_{ll'}{}^{(1)}$ those of order λ, etc.

The diagonal elements of f are solutions of the "generalized transport equation" [KLI, Eq. (119)]

$$C_l{}^{(0)}+C_l'+C_l''+i\sum_{l'}L_{ll'}(f_l-f_{l'})=0, \tag{2.4}$$

where

$$\begin{aligned}C_l'&=C_l{}^{(1)}+\sum_{l'}{}'\left[\frac{\langle C_{ll'}{}^{(0)}H_{l'l}\rangle}{d_{ll'}{}^{-}}-\text{c.c.}\right],\\ C_l''&=C_l{}^{(2)}+\sum_{l'}{}'\left[\frac{\langle C_{ll'}{}^{(1)}H_{l'l}\rangle}{d_{l'l}{}^{-}}-\text{c.c.}\right]\\ &\quad+\sum_{l',l''}{}'\left[\frac{\langle C_{ll''}{}^{(0)}H_{l''l'}H_{l'l}\rangle}{d_{ll'}{}^{-}d_{ll''}{}^{-}}\right.\\ &\quad\left.-\frac{\langle H_{ll''}C_{l''l'}{}^{(0)}H_{l'l}\rangle}{d_{ll'}{}^{-}d_{l''l'}{}^{-}}-\text{c.c.}\right].\end{aligned} \tag{2.5}$$

In (2.5) the angular bracket $\langle\cdots\rangle$ means the *ensemble average*, or the average over the possible positions of all the scattering centers. The quantity $L_{ll'}$ is the "collision operator" and may be written

$$L_{ll'}=L_{ll'}{}^{(0)}+L_{ll'}{}^{(1)}+L_{ll'}{}^{(2)},$$

where

$$L_{ll'}{}^{(0)}=2\pi\delta(\omega_{ll'})\langle|H_{ll'}|^2\rangle, \tag{2.6}$$

$$L_{ll'}{}^{(1)}=2\pi\delta(\omega_{ll'})\sum_{l''}{}'\left[\frac{\langle(ll''l')\rangle}{d_{ll''}{}^{+}}+\frac{\langle(ll'l'')\rangle}{d_{ll''}{}^{-}}\right], \tag{2.7}$$

$$\begin{aligned}L_{ll'}{}^{(2)}&=2\pi\sum_{l'',l'''}{}'\delta(\omega_{ll'})\left(\frac{\langle(ll'''l''l')\rangle}{d_{ll'''}{}^{+}d_{ll''}{}^{+}}\right.\\ &\quad\left.+\frac{\langle(ll'l''l''')\rangle}{d_{ll''}{}^{-}d_{ll'''}{}^{-}}+\frac{\langle(ll''l'l''')\rangle}{d_{ll'''}{}^{-}d_{ll''}{}^{+}}\right)\\ &\quad+\sum_{l''}{}'\left(\frac{\langle|H_{ll''}|^2\rangle\langle|H_{l'l''}|^2\rangle}{d_{ll'}{}^{-}d_{ll''}{}^{-}d_{l'l''}{}^{+}}-\text{c.c.}\right)\\ &\quad+\frac{\langle|H_{ll'}|^2\rangle}{(d_{ll'}{}^{-})^2}(\epsilon_{l'}{}^{(2)*}-\epsilon_l{}^{(2)}-\text{c.c.}).\end{aligned} \tag{2.8}$$

The quantities $(ll'l'')\equiv H_{ll'}H_{l'l''}H_{l''l}$, etc., and the "energy shift" $\epsilon_l{}^{(2)}$ is given by

$$\epsilon_l{}^{(2)}=\sum_{l''}\frac{\langle|H_{ll''}|^2\rangle}{d_{ll''}{}^{+}}. \tag{2.9}$$

As soon as we have solved (2.4), we can obtain the off-diagonal elements of f from (2.1). In order to calculate the current in some direction (say the β direction) we must know the average velocity $\bar{v}_\beta$ in that direction. This is given by

$$\bar{v}_\beta=\text{tr}(fv_\beta), \tag{2.10}$$

where

$$v_\beta=i[H_T,x_\beta], \tag{2.11}$$

the velocity operator. H_T is the total Hamiltonian of the electrons. Since x_β commutes with the potential of the scattering centers and the external electric field,[2] we may write

$$v_\beta=i[H_0,x_\beta], \tag{2.12}$$

where H_0 is the periodic Hamiltonian (which includes the spin-orbit coupling term due to the periodic potential). That is, we may write[3]

$$H_0=p^2/2m+U+(\mathbf{q}\times\nabla U)\cdot\mathbf{p}. \tag{2.13}$$

Here U is the periodic potential, and

$$\mathbf{q}\equiv(1/4m^2c^2)(\mathbf{M}/M_S), \tag{2.14}$$

$\mathbf{M}$ being the magnetization of the sample and M_S the the saturation magnetization. As is well known, the

[2] This would not be true if we included the effect of the spin-orbit coupling due to the scattering potential and the external electric field. The former has been estimated by J. M. Luttinger (unpublished) and by J. Smit, and found to be completely negligible. The latter may be removed by a simple gauge transformation, and has no physical consequences.

[3] R. Karplus and J. M. Luttinger, Phys. Rev. **95**, 1154 (1954).

diagonal elements of (2.12) are given by[4]

$$v_\beta{}^l=\partial\epsilon_l/\partial k_\beta, \tag{2.15}$$

whereas the off-diagonal ones are [KLI Eq. (126)]

$$(v_\beta)_{ll'}=-\omega_{ll'}J_\beta{}^{ll'} \quad (l\neq l'), \tag{2.16}$$

with

$$J_\beta{}^{ll'}=\left(\frac{1}{\omega_c}\int_{\omega_c} w_l{}^*\frac{\partial w_{l'}}{\partial k_\beta}dr\right)\delta_{kk'}. \tag{2.17}$$

Here ω_c is the volume of the unit cell, and w_l is the periodic part of the normalized Block functions of H_0. That is,

$$H_0\psi_l=\epsilon_l\psi_l, \tag{2.18}$$

$$\psi_l=(1/\sqrt{\Omega})e^{ik\cdot r}w_l, \tag{2.19}$$

Ω being the volume of the crystal.

Using these results, we may write the average velocity as a diagonal and an off-diagonal part:

$$\bar{v}_\beta=v_\beta{}^{\mathrm{d}}+v_\beta{}^{\mathrm{o.d.}}, \tag{2.20}$$

$$v_\beta{}^{\mathrm{d}}=\sum_l f_l\partial\epsilon_l/\partial k_\beta=\sum_l f_l v_\beta{}^l, \tag{2.21}$$

$$v_\beta{}^{\mathrm{o.d.}}=+\sum{}'\langle f_{ll'}\rangle\omega_{ll'}J_\beta{}^{l'l}. \tag{2.22}$$

In (2.22) we have replaced $f_{ll'}$ by its ensemble average (since $\omega_{ll'}J_\beta{}^{l'l}$ is independent of the positions of the scattering centers), the justification being exactly the same as that used repeatedly in KLI.

To go further we now have to discuss the matrix elements of H' in some detail, and compute the ensemble averages involved. To make the problem as simple as possible and to avoid extra terms which do not contribute in any essential way to the result, we make the following assumptions about the scattering term H': (a) The scattering centers are located at different lattice points of the crystal. (b) The scattering centers can interpenetrate each other, so that more than one can be at a lattice point. [Assumptions (a) and (b) lead to negligible corrections at low density of scattering centers.] (c) The average periodic part of the scattering potential has been absorbed in the periodic potential U. These assumptions lead to the following expressions for H'

$$H'=\sum_i\varphi(r-r_i)-(N/N_L)\sum_R\varphi(r-R), \tag{2.23}$$

where $\varphi(r)$ is the scattering potential of a single scatterer located at the origin; r_i is a set of N lattice points (N being the number of scattering centers); N_L is the total number of lattice points, and the sum over R is a sum over all lattice points. Assumption (b) then allows the possibility of some of the r_i being equal. The matrix elements of H' are given by

$$H_{ll'}=\varphi_{ll'}\left[\sum_{r_i}e^{-i(k-k')\cdot r_i}-\frac{N}{N_L}\sum_R e^{-i(k-k')\cdot R}\right], \tag{2.24}$$

where

$$\varphi_{ll'}=\int_\Omega\psi_l{}^*\varphi(r)\psi_{l'}dr. \tag{2.25}$$

From (2.24) we have at once that

$$(H')_{nk,\,n'k}=\varphi_{nk,\,n'k}\left[N-\frac{N}{N_L}N_L\right]=0. \tag{2.26}$$

If $k\neq k'$ the second term of (2.24) is zero (since k and k' extend over a Brillouin zone) and we have

$$H_{ll'}=\varphi_{ll'}\sum_{r_i}e^{-i(k-k')\cdot r_i}, \quad (k\neq k'). \tag{2.27}$$

We consider first the off-diagonal contribution to the velocity. Since $J_\beta{}^{ll'}$ contains the factor $\delta_{kk'}$, we need $\langle f_{ll'}\rangle$ for $k=k'$. By (2.26), $f_{nk,\,nk'}{}^{(-1)}$ vanishes. To calculate $f_{nk,\,nk'}{}^{(0)}$ we need, for $k''\neq k$,

$$\langle(H')_{nk,\,l''}(H')_{l'',\,n'k}\rangle=N\varphi_{nk,\,l''}\varphi_{l'',\,n'k}. \tag{2.28}$$

Therefore, since $C_{ll'}{}^{(0)}$ is independent of the positions of the scatterers,

$$\langle f_{ll'}{}^{(0)}\rangle_{k=k'}=\frac{1}{d_{ll'}{}^-}\times\left[C_{ll'}{}^{(0)}+N\sum_{l''}{}'\varphi_{ll''}\varphi_{l''l'}\left(\frac{f_l-f_{l''}}{d_{ll''}{}^-}-\frac{f_{l''}-f_{l'}}{d_{l''l'}{}^-}\right)\right]_{k=k'}. \tag{2.29}$$

The off-diagonal contribution to the velocity is

$$v_\beta{}^{\mathrm{o.d.}}=\sum_{l,l'}{}'C_{ll'}{}^{(0)}J_\beta{}^{l'l}+N\sum_{l,l',l''}{}'\varphi_{ll''}\varphi_{l''l'}\left(\frac{f_l-f_{l''}}{d_{ll''}{}^-}-\frac{f_{l''}-f_{l'}}{d_{l''l'}{}^-}\right)J_\beta{}^{l'l}. \tag{2.30}$$

In (2.30) we have put $\omega_{nk,\,n'k}/d_{nk,\,n'k}=1$, which assumes that there is no accidental degeneracy (i.e., that $\epsilon_{nk}\neq\epsilon_{n'k}$ for $n\neq n'$).

The first term of (2.30) is easily calculated. For this purpose we need the matrix elements of C. From KLI, Eq. (113), these are given by

$$C_{ll'}=ieE_\alpha\left[\left(\frac{\partial}{\partial k_\alpha}+\frac{\partial}{\partial k_\alpha{}'}\right)\right]\rho_{ll'}+\sum_{l''}(J_\alpha{}^{ll''}\rho_{l''l'}-\rho_{ll''}J_\alpha{}^{l''l'}). \tag{2.31}$$

To the lowest order in λ, $\rho^{(0)}=\rho(H_0)$, so that

$$\rho_{ll'}{}^{(0)}=\rho(\epsilon_l)\delta_{ll'}=\rho_l\delta_{nn'}\delta_{kk'}. \tag{2.32}$$

Therefore, for $l\neq l'$,

$$C_{ll'}{}^{(0)}=-ieE_\alpha(\rho_l-\rho_{l'})J_\alpha{}^{ll'}. \tag{2.33}$$

[4] See reference 3, Appendix C.

The first term of (2.30) then becomes

$$\sum_{l,l'} C_{ll'}{}^{(0)} J_\beta{}^{l'l} = -ieE_\alpha \sum_{l,l'} (\rho_l - \rho_{l'}) J_\alpha{}^{ll'} J_\beta{}^{l'l}$$

$$= -ieE_\alpha \sum_l \rho_l \sum_{l'} (J_\alpha{}^{ll'} J_\beta{}^{l'l} - J_\beta{}^{ll'} J_\alpha{}^{l'l})$$

$$= -ieE_\alpha \sum_l \rho_l \left(\frac{\partial J_\alpha{}^l}{\partial k_\beta} - \frac{\partial J_\beta{}^l}{\partial k_\alpha} \right), \tag{2.34}$$

on making use of (2.17) of Karplus and Luttinger.[3] The terms (2.34) were already present in the original paper of Karplus and Luttinger,[4] and are also found in KLI.[5]

The second term of (2.30) may also be put in somewhat simpler form by permuting a few of the l indices. We have

$$\sum_{l',l'',l'}{}' \varphi_{ll''} \varphi_{l''l'} \left(\frac{f_l - f_{l''}}{d_{ll''}^-} - \frac{f_{l''} - f_{l'}}{d_{l''l'}^-} \right) J_\alpha{}^{l'l}$$

$$= \sum_{l,l'l''}{}' f_l \left[\frac{\varphi_{ll'} (\varphi_{l'l''} J_\beta{}^{l''l} - J_\beta{}^{l'l''} \varphi_{l''l})}{d_{ll'}^-} + \text{c.c.} \right]$$

$$= \sum_{l'l,} f_l \left(\frac{\varphi_{ll'} (\varphi, J_\beta)_{l'l}}{d_{ll'}^-} + \text{c.c.} \right)$$

$$\div \sum_{l,l'} f_l \left(\frac{|\varphi_{ll'}|^2 (J_\beta{}^l - J_\beta{}^{l'})}{d_{ll'}^-} + \text{c.c.} \right). \tag{2.35}$$

The last term arises because we have allowed index equalities on the $J^{ll'}$ in order to write the commutator (φ, J). [The other restrictions on index equalities have been dropped since they exclude only single k values, and therefore give rise to terms which are $O(1/\Omega)$.] Now from (2.31), if we let ρ be an arbitrary function (Q) of the coordinates, we get

$$(Q, J_\alpha)_{ll'} = D_\alpha Q_{ll'}, \tag{2.36}$$

where

$$D_\alpha = \frac{\partial}{\partial k_\alpha} + \frac{\partial}{\partial k_\alpha'}, \tag{2.37}$$

since x_α commutes with Q. Therefore (2.30) becomes

$$v_\beta{}^{\text{o.d.}} = ieE_\alpha \sum_l \rho_l \left(\frac{\partial J_\beta{}^l}{\partial k_\alpha} - \frac{\partial J_\alpha{}^l}{\partial k_\beta} \right) + N \sum_l f_l{}^{(0)} \sum_{l'}$$

$$\times \left(\frac{\varphi_{ll'} D_\beta \varphi_{l'l} - |\varphi_{ll'}|^2 (J_\beta{}^l - J_\beta{}^{l'})}{d_{ll'}^-} + \text{c.c.} \right). \tag{2.38}$$

Since we are interested in $v_\beta{}^{\text{o.d.}}$ to order λ^0, f_l in (2.38) has been replaced by its lowest order $f_l{}^{(0)}$. That is, we may write

$$f_l = f_l{}^{(0)} + f_l{}^{(1)} + f_l{}^{(2)}, \tag{2.39}$$

where $f_l{}^{(0)}$ is of order λ^{-2}, $f_l{}^{(1)}$ is of order λ^{-1}, etc. Then from (2.4), (2.6), (2.28), (2.31), and (2.32), $f_l{}^{(0)}$ satisfies the *ordinary* transport equation[6]

$$eE_\alpha \frac{\partial \rho_l}{\partial k_\alpha} + N \sum_{l'} 2\pi \delta(\omega_{ll'}) |\varphi_{ll'}|^2 (f_l{}^{(0)} - f_{l'}{}^{(0)}) = 0. \tag{2.40}$$

In addition to the contribution (2.38) of order λ^0, there is also a contribution of the same order from $f_l{}^{(2)}$ (as well as one of order λ^{-1} from $f_l{}^{(1)}$). To obtain these contributions it is necessary to solve the generalized transport equation (2.4). It is convenient in solving (2.4) to divide the corrections to $f_l{}^{(0)}$ into two classes, which we shall call "field corrections" and "collision corrections." The former arise from the C_l' and C_l'' terms of (2.4), the latter from $L_{ll'}{}^{(1)}$ and $L_{ll'}{}^{(2)}$. As we shall see below, to the order in which we are working these terms give additive corrections.

We first consider the field terms. In order to obtain C_l' and C_l'' we need $C_l{}^{(1)}$ and $C_l{}^{(2)}$. These are given by (2.31), as soon as we know the expansion of ρ in powers of λ. This is given by[7]

$$\rho_{ll'} = \rho_{ll'}{}^{(0)} + \rho_{ll'}{}^{(1)} + \rho_{ll'}{}^{(2)}, \tag{2.41}$$

$$\rho_{ll'}{}^{(0)} = \rho_l \delta_{ll'}, \tag{2.42}$$

$$\rho_{ll'}{}^{(1)} = \frac{\rho_l - \rho_{l'}}{\omega_{ll'}} H_{ll'}', \tag{2.43}$$

$$\rho_{ll'}{}^{(2)} = \gamma \rho_l \delta_{ll'} + \sum_{l''} \frac{H_{ll''}' H_{l''l'}'}{\omega_{l'l''}} \times \left[\frac{\rho_l - \rho_{l'}}{\omega_{ll'}} - \frac{\rho_l - \rho_{l''}}{\omega_{ll''}} \right], \tag{2.44}$$

$$\gamma \equiv \sum_{l,l'} \frac{\langle |H_{ll'}'|^2 \rangle}{\omega_{ll'}} \left[\frac{\rho_l - \rho_{l'}}{\omega_{ll'}} - \frac{\partial \rho_l}{\partial \epsilon_l} \right]. \tag{2.45}$$

Inserting these in (2.31) and making use of (2.5) and the ensemble average theorem, we obtain, after some

[5] Equation (135). The sign in KLI is wrong, due to sign error carried over from Eq. (134) of that paper.

[6] The solution of (2.40) is not unique, since we may add to any solution an arbitrary function of ϵ_l and get a new solution. This causes no difficulty in the usual transport theory, since such a term is easily seen to give no contribution to (2.21) in any case. However, such a term might give a contribution to (2.38), and it must be discussed more carefully. The simplest way to eliminate this ambiguity it to note that, for a crystal, f_l must be an invariant under the crystal group if the electric field is simultaneously transformed. However, from E_α and ϵ_l (which is already invariant) one cannot construct a term linear in E_α which is invariant, so that an f_l with the correct transformation properties does not have this ambiguity. If the sample has a magnetization $\mathbf{M}$, a term of the for $\mathbf{E} \cdot \mathbf{M}$ can be formed. This cannot give rise to an anomalous Hall effect, however, since it vanishes for $\mathbf{M}$ perpendicular to $\mathbf{E}$.

[7] KLI, Appendix C. It is simply necessary to write l instead of k, and to rewrite the formulas in terms of ρ_l rather than the explicit exponential distribution used there.

algebra,

$$C_l'=0, \tag{2.46}$$

$$C_{l''}=ieE_\alpha\left[\gamma\frac{\partial\rho_l}{\partial k_\alpha}+\frac{\partial\rho_l^{(2)}}{\partial k_\alpha}+N\sum_{l'}\left\{\frac{1}{d_{ll'}^-}[(\varphi_{l'l}D_\alpha\varphi_{ll'})+|\varphi_{ll'}|^2(J_\alpha{}^l-J_\alpha{}^{l'})]\frac{\rho_l-\rho_{l'}}{\omega_{ll'}}+\text{c.c.}\right\}\right.$$

$$\left.+N\sum_{l'}\left\{\frac{|\varphi_{ll'}|^2}{d_{ll'}^-}D_\alpha\left(\frac{\rho_l-\rho_{l'}}{\omega_{ll'}}\right)+\text{c.c.}\right\}\right], \tag{2.47}$$

where

$$\rho_l^{(2)}=N\sum_{l'}\frac{|\varphi_{ll'}|^2}{\omega_{ll'}}\left[\frac{\partial\rho_l}{\partial\epsilon_l}-\frac{\rho_l-\rho_{l'}}{\omega_{ll'}}\right]. \tag{2.48}$$

Since C_l' vanishes, there are only λ^2 corrections to the field terms. Therefore if we want f_l corrections to the second order we get independent contributions from the field terms and the collision terms. More formally, let us introduce

$$f_l=f_l{}^F+f_l{}^C, \tag{2.49}$$

where $f_l{}^F$ is $O(\lambda^0)$. Insert this in (2.4) dropping contributions of higher order than λ^2: if we choose $f_l{}^F$ to satisfy

$$C_l''+i\sum_{l'}L_{ll'}{}^{(0)}(f_l{}^F-f_{l'}{}^F)=0, \tag{2.50}$$

we find that

$$C_l{}^{(0)}+i\sum_{l'}L_{ll'}(f_l{}^C-f_{l'}{}^C)=0. \tag{2.51}$$

That is, the field correction $f_l{}^F$ satisfies the lowest order transport equation with C_l'' as driving term instead of $C_l{}^{(0)}$. Further if we write for the "collision contribution" $f_l{}^C$ an expansion in λ,

$$f_l{}^C=f_l{}^{(0)}+f_l'+f_l'', \tag{2.52}$$

and insert this in (2.51), we get on equating equal powers of λ

$$\sum_{l'}L_{ll'}{}^{(1)}(f_l{}^{(0)}-f_{l'}{}^{(0)})+\sum_{l'}L_{ll'}{}^{(0)}(f_l'-f_{l'}')=0, \tag{2.53}$$

$$\sum_{l'}L_{ll'}{}^{(2)}(f_l{}^{(0)}-f_{l'}{}^{(0)})+\sum_{l'}L_{ll'}{}^{(1)}(f_l'-f_{l'}')+\sum_{l'}L_{ll'}{}^{(0)}(f_l''-f_{l'}'')=0. \tag{2.54}$$

Since $f_l{}^{(0)}$ is known, in principle, from (2.40), it may be inserted in (2.53), giving again the usual transport equation for f_l', except with a different driving term. Similarly, since $f_l{}^{(0)}$ and f_l' are known, (2.54) becomes an "ordinary" transport equation for f_l''.

Finally, for completeness, we give the ensemble averages which are necessary to make the collision operators $L_{ll'}{}^{(1)}$ and $L_{ll'}{}^{(2)}$ explicit. These are, from (2.7) and (2.8),

$$\langle(ll'l'')\rangle=N\varphi_{ll'}\varphi_{l'l''}\varphi_{l''l}, \tag{2.55}$$

$$\langle(ll'l''l''')\rangle=\varphi_{ll'}\varphi_{l'l''}\varphi_{l''l'''}\varphi_{l'''l}\times[N+N(N-1)\delta_{k-k'+k''-k''',0}], \tag{2.56}$$

for all the k indices unequal. They vanish whenever any of the k indices are equal. The δ function in (2.56) is to be interpreted as giving something whenever $k-k'+k''-k'''=0$ *modulo* a reciprocal lattice vector.

3. HALL EFFECT ARISING FROM SPIN-ORBIT COUPLING

The general formulas of Sec. II enable us to calculate the corrections to the conductivity to order λ^2. We are not interested in this paper in the general problem, but only in the problem of whether a transverse current exists, i.e., in the Hall effect. Now for isotropic scatterers it is easy to see that there is no transverse current unless there is spin-orbit coupling. The spin-orbit coupling is small, in general, and therefore the transverse current will be proportional to it and thus [from (2.13) and (2.14)] to the magnetization. Therefore, to study the anomalous Hall effect we shall study that contribution to the average velocity which is of the first order in the spin-orbit coupling.

We begin with the discussion of the lowest-order velocity (of order λ^{-2}) which is given by $f_l{}^{(0)}$ from (2.40) in connection with (2.21). Since the spin-orbit coupling does not affect the energy to first order (see Appendix B), the velocity operator in (2.21) and the distribution function ρ_l in (2.40) are not affected by it. The only thing which might be affected is the matrix element of the scattering potential. This we write as

$$\varphi_{ll'}=\varphi_{ll'}{}^{(0)}+\varphi_{ll'}{}^{(1)}, \tag{3.1}$$

where $\varphi_{ll'}{}^{(1)}$ represents the first-order correction due to spin-orbit coupling. Therefore

$$|\varphi_{ll'}|^2=|\varphi_{ll'}{}^{(0)}|^2+\varphi_{ll'}{}^{(0)}\varphi_{l'l}{}^{(1)}+\varphi_{ll'}{}^{(1)}\varphi_{l'l}{}^{(0)}=|\varphi_{ll'}{}^{(0)}|^2+\varphi_{ll'}{}^{(0)}\varphi_{l'l}{}^{(1)}+(\varphi_{ll'}{}^{(0)}\varphi_{l'l}{}^{(1)})^*. \tag{3.2}$$

However [by Appendix B, (B.7) and (B.12)],

$$(\varphi_{ll'}{}^{(0)})^*=\delta_n\delta_{n'}\varphi_{ll'}{}^{(0)}, \tag{3.3}$$

$$(\varphi_{ll'}{}^{(1)})^*=-\delta_n\delta_n\varphi_{l'l}{}^{(1)}, \tag{3.4}$$

where $\delta_n=\pm1$. Thus the third term of (3.2) is equal and opposite to the second, and we have

$$|\varphi_{ll'}|^2=|\varphi_{ll'}{}^{(0)}|^2. \tag{3.5}$$

Therefore, there is *no* effect of spin-orbit coupling and *no* anomalous Hall effect, to order λ^{-2}. The quantity $f_l{}^{(0)}$ has no correction to the first order in the spin-orbit coupling.

Next we consider the corrections of order λ^{-1}. They

arise from the correction f_l' [given by (2.53)] in connection with (2.21). In order to obtain f_l' to first order in the spin-orbit coupling we need to expand $L_{ll'}{}^{(1)}$. From (2.1) and (2.55), this is

$$L_{ll'}{}^{(1)}=2\pi N\delta(\omega_{ll'})\sum_{l''}\left[\frac{\varphi_{ll'}\varphi_{l'l''}\varphi_{l''l}}{d_{ll''}{}^{-}}+\text{c.c.}\right], \quad (3.6)$$

$$\varphi_{ll'}\varphi_{l'l''}\varphi_{l''l}=\varphi_{ll'}{}^{(0)}\varphi_{l'l''}{}^{(0)}\varphi_{l''l}{}^{(0)} +(\varphi_{ll'}{}^{(1)}\varphi_{l'l''}{}^{(0)}\varphi_{l''l}{}^{(0)}+\text{cyclic}). \quad (3.7)$$

Using (3.3) and (3.4) we see that the zeroth-order term is real, while the first-order term is pure imaginary. By means of the well known relationship (as s goes to zero)

$$1/d_{ll'}{}^{-}=\mathrm{P}(1/\omega_{ll'})+i\pi\delta(\omega_{ll'}), \quad (3.8)$$

(where P indicates principal value), we may write

$$L_{ll'}{}^{(1)}=L_{ll'}{}^{(10)}+L_{ll'}{}^{(11)}, \quad (3.9)$$

where

$$L_{ll'}{}^{(10)}=4\pi N\delta(\omega_{ll'})\sum_{l''}\mathrm{P}\frac{\varphi_{ll'}{}^{(0)}\varphi_{l'l''}{}^{(0)}\varphi_{l''l}{}^{(0)}}{\omega_{ll''}}, \quad (3.10)$$

$$L_{ll'}{}^{(11)}=(2\pi)^2Ni\delta(\omega_{ll'})\sum_{l''}\delta(\omega_{ll''}) \times(\varphi_{ll'}{}^{(1)}\varphi_{l'l''}{}^{(0)}\varphi_{l''l}{}^{(0)}+\text{cyclic}). \quad (3.11)$$

Writing correspondingly

$$f_l'=f_l{}^{(10)}+f_l{}^{(11)}, \quad (3.12)$$

$f_l{}^{(11)}$ being the first-order correction in the spin-orbit coupling, (2.53) becomes equivalent to

$$\sum_{l'}L_{ll'}{}^{(10)}(f_l{}^{(0)}-f_{l'}{}^{(0)}) +\sum_{l'}2\pi N\delta(\omega_{ll'})|\varphi_{ll'}{}^{(0)}|^2(f_l{}^{(10)}-f_{l'}{}^{(10)}), \quad (3.13)$$

and

$$\sum_{l'}L_{ll'}{}^{(11)}(f_l{}^{(0)}-f_{l'}{}^{(0)}) +\sum_{l'}2\pi N\delta(\omega_{ll'})|\varphi_{ll'}{}^{(0)}|^2(f_l{}^{(11)}-f_{l'}{}^{(11)}). \quad (3.14)$$

The Hall current is contained in $f_l{}^{(11)}$ and not in $f_l{}^{(10)}$, and therefore it is obtained by solving (3.14). Until we make some assumptions about the scattering potential φ and the Bloch functions we cannot solve (3.14), since it is in general an *integral equation* for $f_l{}^{(11)}$ [just as (2.40) is an integral equation for $f_l{}^{(0)}$], and cannot be solved explicitly. We shall return to these questions in the next section, but shall now proceed to a similar reduction of the spin-orbit contribution for the next order in λ.

The average velocity to order λ^0 is composed of three parts: (1) the off-diagonal contribution (2.38); (2) the diagonal contribution due to the "field correction" ($f_l{}^F$), calculated from (2.50); (3) the diagonal contribution due to the "collision correction" (f_l''), calculated from (2.54). We consider these in turn.

(1) Making use of (3.3) and (3.4) again, remembering (see Appendix B) that $J_\beta{}^l$ is pure imaginary and of first order in the spin-orbit coupling, the spin-orbit part of (2.38) becomes

$$v_\beta{}^{\text{o.d.}}=ieE_\alpha\sum_l\rho_l\left(\frac{\partial J_\beta{}^l}{\partial k_\alpha}-\frac{\partial J_\alpha{}^l}{\partial k_\beta}\right)-\sum_l f_l{}^{(0)}w_\beta{}^l -2\pi Ni\sum_l f_l{}^{(0)}\sum_{l'}\delta(\omega_{ll'})|\varphi_{ll'}{}^{(0)}|^2(J_\beta{}^l-J_\beta{}^{l'}), \quad (3.15)$$

where

$$w_\beta{}^l=2\pi N\sum_{l'}\delta(\omega_{ll'})\,\mathrm{Im}(\varphi_{ll'}D_\beta\varphi_{l'l}). \quad (3.16)$$

In (3.16), Im means the imaginary part of what follows. We may also write

$$\mathrm{Im}(\varphi_{ll'}D_\alpha\varphi_{l'l}) =(1/i)[\varphi_{ll'}{}^{(0)}D_\alpha\varphi_{l'l}{}^{(1)}+\varphi_{ll'}{}^{(1)}D_\alpha\varphi_{l'l}{}^{(0)}]. \quad (3.17)$$

The last term of (3.15) may be transformed:

$$2\pi Ni\sum_l f_l{}^{(0)}\sum_{l'}\delta(\omega_{ll'})|\varphi_{ll'}{}^{(0)}|^2(J_\beta{}^l-J_\beta{}^{l'}) =2\pi Ni\sum_{l,l'}\delta(\omega_{ll'})|\varphi_{ll'}{}^{(0)}|^2(f_l{}^{(0)}-f_{l'}{}^{(0)})J_\beta{}^l =-ieE_\alpha\sum_l\frac{\partial\rho_l}{\partial k_\alpha}J_\beta{}^l=ieE_\alpha\sum_l\rho_l\frac{\partial J_\beta{}^l}{\partial k_\alpha}, \quad (3.18)$$

where we have made use of the transport equation (2.40), and (3.5). Therefore

$$v_\beta{}^{\text{o.d.}}=-ieE_\alpha\textstyle\sum_l\rho_l\partial J_\alpha{}^l/\partial k_\beta-\sum_l f_l{}^{(0)}w_\beta{}^l. \quad (3.19)$$

(2) For (2.50) we need the spin-orbit part of C_l''. From (2.47), (3.3), and (3.4), we see that the only part of C_l'' which gives a first-order spin-orbit correction is

$$C_l''=ieE_\alpha\{\rho_l'w_\alpha{}^l+2\pi Ni\textstyle\sum_{l'}\rho_{l'}'\delta(\omega_{ll'}) \times|\varphi_{ll'}{}^{(0)}|^2(J_\alpha{}^l-J_\alpha{}^{l'})\}, \quad (3.20)$$

$$\rho_l'=\partial\rho_l/\partial\epsilon_l. \quad (3.21)$$

The second term of (3.20) gives a contribution to $f_l{}^F$ which can be obtained explicitly. Writing

$$f_l{}^F=g_l-ieE_\alpha\rho_l'J_\alpha{}^l, \quad (3.22)$$

we see from (2.50) that the equation for g_l is simply

$$eE_\alpha\rho_l'w_\alpha{}^l+2\pi N\textstyle\sum_{l'}|\varphi_{ll'}{}^{(0)}|^2\delta(\omega_{ll'})(g_l-g_{l'})=0. \quad (3.23)$$

The contribution to the current is, from (2.21),

$$v_\beta{}^F=\sum_l f_l{}^Fv_\beta{}^l=\sum_l g_lv_\beta{}^l-ieE_\alpha\sum_l\rho_l'J_\alpha{}^l\frac{\partial\epsilon_l}{\partial k_\beta} =\sum_l g_lv_\beta{}^l+ieE_\alpha\sum_l\rho_l\frac{\partial J_\alpha{}^l}{\partial k_\beta}. \quad (3.24)$$

If we call

$$u_\beta=v_\beta{}^{\text{o.d.}}+v_\beta{}^F, \quad (3.25)$$

then

$$u_\beta=\textstyle\sum_l(g_lv_\beta{}^l-f_l{}^{(0)}w_\beta{}^l). \quad (3.26)$$

We may write the equation for $f_l^{(0)}$ as

$$eE_\alpha\rho_l' v_\alpha{}^l + 2\pi N \sum_{l'} |\varphi_{ll'}{}^{(0)}|^2 \times\delta(\omega_{ll'})(f_l^{(0)}-f_{l'}{}^{(0)})=0. \quad (3.27)$$

Comparing (3.23), (3.27), and (3.26), we see that there is a high degree of symmetry between $v_\alpha{}^l$ and $w_\alpha{}^l$ in our final expression.

(3) To obtain the spin-orbit part of f_l'' we must expand (2.54) to the first order in the spin-orbit coupling. Writing

$$\begin{aligned} L_{ll'}{}^{(1)} &= L_{ll'}{}^{(10)}+L_{ll'}{}^{(11)}, \\ L_{ll'}{}^{(2)} &= L_{ll'}{}^{(20)}+L_{ll'}{}^{(21)}, \\ f_l' &= f_l^{(10)}+f_l^{(11)}, \\ f_l'' &= f_l^{(20)}+f_l^{(21)} \end{aligned} \quad (3.28)$$

(where the second term on the right-hand side is always the spin-orbit correction), the equation for $f_l^{(21)}$ becomes

$$\begin{aligned} &\sum_{l'}[L_{ll'}{}^{(21)}(f_l^{(0)}-f_{l'}{}^{(0)}) \\ &\quad +L_{ll'}{}^{(10)}(f_l^{(11)}-f_{l'}{}^{(11)})+L_{ll'}{}^{(11)}(f_l^{(10)}-f_{l'}{}^{(10)})] \\ &\quad +2\pi N\sum_{l'}|\varphi_{ll'}{}^{(0)}|^2\delta(\omega_{ll'})(f_l^{(21)}-f_{l'}{}^{(21)})=0. \end{aligned} \quad (3.29)$$

The only new element in (3.29) is $L_{ll'}{}^{(21)}$. From (2.8), (2.56), (3.3), and (3.4), and a little algebra, this is

$$L_{ll'}{}^{(21)} = (2\pi i)^2 N\delta(\omega_{ll'}) \times \sum_{l'',l'''} \delta(\omega_{ll''})\, \mathrm{P}\left(\frac{1}{\omega_{ll'''}}\right)\{\}, \quad (3.30)$$

$$\begin{aligned} \{\} = \mathrm{Im}\{ &\varphi_{ll'}\varphi_{l'l''}\varphi_{l''l'''}\varphi_{l'''l}(1+N\delta_{k-k'+k''-k''',0}) \\ &+\varphi_{ll'}\varphi_{l'l'''}\varphi_{l'''l''}\varphi_{l''l}(1+N\delta_{k-k'+k'''-k'',0}) \\ &+\varphi_{ll'''}\varphi_{l'''l'}\varphi_{l'l''}\varphi_{l''l}(1+N\delta_{k+k'-k''-k''',0})\}. \end{aligned} \quad (3.31)$$

After we have solved (3.29), we obtain a velocity contribution of order λ^0 from

$$v_\beta{}^{(21)} = \sum_l f_l^{(21)} v_\beta{}^l. \quad (3.32)$$

It is again impossible to proceed any further without some knowledge of the scattering potential and the Bloch functions.

4. CALCULATION OF HALL EFFECT IN "EFFECTIVE MASS" LIMIT

In order to deal with the extremely complicated formulas of the previous section, it is necessary to introduce some rather drastic simplifications. These will give us a result which is a rigorous consequence of our theory, though it will not be relevent (except as an extremely crude estimate) to the situation in real ferromagnetic substances like Fe or Ni. However, we view the main purpose of this paper as being to exhibit the structure of the different terms which come into the Hall effect (rather than to make a realistic computation of its value), so that this will not bother us too much. Further, so little is known about the real Bloch functions of a ferromagnetic substance that a realistic computation seems impossible in any case.

We therefore consider the following limit, which we shall call the "effective mass" limit.

(a) We assume that there are few electrons in the magnetic band, and that they are at absolute zero of temperature. This means that the unperturbed distribution function ρ_l is a step function

$$\begin{aligned} \rho_l &= \text{const}, \quad \epsilon_l < \epsilon_F \\ &= 0, \quad\quad \epsilon_l > \epsilon_F, \end{aligned} \quad (4.1)$$

where the Fermi level ϵ_F is very small compared to the band width. We assume it to be so small that we may write for any ϵ_l which occurs in ρ_l the effective-mass expression

$$\epsilon_l = k^2/2m^*, \quad (4.2)$$

where m^* is the effective mass of the electrons in the band n.

(b) We assume that the scattering potential is very slowly varying over a unit cell. More analytically, we shall assume that φ has *no* Fourier components which are of the order of a reciprocal lattice vector. From Appendix C, it then follows that the matrix element $\varphi_{ll'}$ is given by an expansion of the type

$$\varphi_{ll'} = \varphi_{kk'}[\delta_{nn'}+(k_\mu'-k_\mu)J_\mu{}^{nn'}(k) +\tfrac{1}{2}(k_\mu'-k_\mu)(k_\nu'-k_\nu)J_{\mu\nu}{}^{nn'}(k)+\cdots], \quad (4.3)$$

where $\varphi_{kk'}$ is the ordinary plane-wave matrix element, and the J's are defined in Appendix C.

This expression will be used as follows. In computing any of the different contributions to the velocity which arise, we shall only take enough terms of (4.3) so as to give the first nonvanishing result. At the end of the calculation we shall see that in fact each of these contributions has a very similar structure.

With these assumptions we have at once that, to the approximation in which we are working,

$$|\varphi_{ll'}|^2 = \varphi_{kk'}{}^2\delta_{nn'}. \quad (4.4)$$

Therefore, the lowest order transport equation (3.27) becomes

$$eE_\alpha\rho_{nk}'v_\alpha{}^{nk}+2\pi N\sum_{k'}\varphi_{kk'}{}^2\delta(\epsilon_{nk}-\epsilon_{nk'}) \times(f_{nk}{}^{(0)}-f_{nk'}{}^{(0)}). \quad (4.5)$$

From assumption (a), ρ_l' is a rotational invariant and $v_\alpha{}^{nk}$ is proportional to k_α. Therefore we may solve this equation in the usual way,

$$f_{nk}{}^{(0)} = -\tau_0 eE_\alpha\rho_{nk}'v_\alpha{}^{nk}, \quad (4.6)$$

where the "relaxation time" τ_0 is given by

$$\tau_0 = \left[\frac{4\pi^2}{n\int\varphi^2(k-k')\delta(\epsilon_{nk}-\epsilon_{nk'})[1-\cos(k,k')]dk'}\right]_{k=k_F}. \quad (4.7)$$

The n in front of the integral is the density of scattering centers.

It is convenient to make still another assumption in evaluating integrals such as occur in (4.7). That is, we assume that the range of the potential (say r_0) is small enough so that

$$k_F r_0 \ll 1. \tag{4.8}$$

The integral in (4.7) becomes

$$\bar{\varphi}^2\left(\int \delta(\epsilon_{nk}-\epsilon_{nk'})dk'\right)_{k=k_F} = \bar{\varphi}^2(2\pi)(2m^*)^{\frac{3}{2}}(\epsilon_F)^{\frac{1}{2}}, \tag{4.9}$$

where

$$\bar{\varphi}=\int \varphi(r)dr. \tag{4.10}$$

In this approximation, (4.7) is

$$\tau_0^{-1}=n\bar{\varphi}^2(2m^*)^{\frac{3}{2}}(\epsilon_F)^{\frac{1}{2}}/2\pi. \tag{4.11}$$

We now compute the velocity contribution of order λ^{-1}. For this we need $L_{ll'}{}^{(11)}$ to insert in (3.14). From (3.11),

$$L_{ll'}{}^{(11)} = -(2\pi)^2 N\delta(\omega_{ll'})\sum_{l''}\delta(\omega_{ll''}) \times \mathrm{Im}(\varphi_{ll'}\varphi_{l'l''}\varphi_{l''l}). \tag{4.12}$$

The δ functions in (4.12) insure the equality of the indices n, n', n'', unless the band is degenerate at $k=0$, which we specifically exclude. Then, from (4.3) and (C.7), we have

$$\mathrm{Im}(\varphi_{ll'}\varphi_{l'l''}\varphi_{l''l}) = \frac{i}{2}\varphi_{kk'}\varphi_{k'k''}\varphi_{k''k}(k_\mu'-k_\mu'')(k_\nu'-k_\nu)\left(\frac{\partial J_\mu{}^l}{\partial k_\nu}-\frac{\partial J_\nu{}^l}{\partial k_\mu}\right). \tag{4.13}$$

Putting (4.13) in (4.12) and making the same approximations as before, we obtain

$$L_{ll'}{}^{(11)}=\frac{i\pi^2 n\bar{\varphi}^3\left[(2m^*)^{\frac{3}{2}}(\epsilon_l)^{\frac{1}{2}}\right]\delta(\omega_{ll'})}{(2\pi)^2\Omega} \times(k_\mu' k_\nu - k_\mu k_\nu')\left(\frac{\partial J_\mu{}^l}{\partial k_\nu}-\frac{\partial J_\nu{}^l}{\partial k_\mu}\right). \tag{4.14}$$

Then

$$\sum_{l'} L_{ll'}{}^{(11)}(f_1{}^{(0)}-f_{l'}{}^{(0)}) = +\frac{in\bar{\varphi}^3\epsilon_F\tau_0}{3}\left[\frac{(2m^*)^{\frac{3}{2}}\epsilon_F{}^{\frac{1}{2}}}{2\pi}\right]^2 \times\rho_l' eE_\alpha k_\nu\left(\frac{\partial J_\alpha{}^l}{\partial k_\nu}-\frac{\partial J_\nu{}^l}{\partial k_\alpha}\right)_0, \tag{4.15}$$

where the subscript zero on the last term means that we are taking the quantity for $k=0$, which is consistent with all the expansions that we have made. The expression (4.15) is exactly of the same structure in its k k dependence as the driving term of the zeroth order transport equation. Therefore we can solve it at once with the relaxation time τ_0,

$$f_l{}^{(11)}=-ieE_\alpha\left(\frac{\partial J_\alpha{}^l}{\partial k_\nu}-\frac{\partial J_\nu{}^l}{\partial k_\alpha}\right)_0 k_\nu\rho_l'\frac{i\epsilon_F}{3n\bar{\varphi}}. \tag{4.16}$$

This gives rise to an average velocity

$$v_\beta{}^{(11)}=-ieE_\alpha\left(\frac{\partial J_\beta{}^l}{\partial k_\alpha}-\frac{\partial J_\alpha{}^l}{\partial k_\beta}\right)_0\frac{\epsilon_F}{3n\bar{\varphi}}. \tag{4.17}$$

We consider next the velocity contribution of order λ^0. There are two contributions: u_β from (3.26), and $v_\beta{}^{(21)}$ from (3.32). We begin with u_β, which requires the calculation of $w_\alpha{}^l$, from (3.16). Using (4.3) we have

$$\mathrm{Im}(\varphi_{ll'}D_\alpha\varphi_{l'l})=\frac{1}{i}\varphi_{kk'}{}^2(k_\mu-k_\mu')\frac{\partial J_\mu{}^l}{\partial k_\alpha}\delta_{nn'}+\cdots. \tag{4.18}$$

Inserting the leading term of (4.18) in (3.16), and doing all the integration just as before, we find

$$w_\alpha{}^l=\frac{1}{i}\frac{1}{\tau_0}\left(\frac{\partial J_\mu{}^l}{\partial k_\alpha}\right)_0 k_\mu. \tag{4.19}$$

Since $w_\alpha{}^l$ is proportional to k_μ, we can integrate (3.23) with the relaxation time τ_0, i.e.,

$$g_l=-\tau_0 eE_\alpha\rho_l' w_\alpha{}^l=ieE_\alpha\left(\frac{\partial J_\mu{}^l}{\partial k_\alpha}\right)_0 k_\mu\rho_l'. \tag{4.20}$$

Finally, from (3.26), using (4.20), (4.19), and (4.6), we obtain

$$u_\beta=-ieE_\alpha\left(\frac{\partial J_\beta{}^l}{\partial k_\alpha}-\frac{\partial J_\alpha{}^l}{\partial k_\beta}\right)_0. \tag{4.21}$$

This result has the remarkable property (just as did the original result of Karplus and Luttinger) that it is independent of any properties of the scattering mechanism.

We come finally to the collision correction $v_\beta{}^{(21)}$, for which we must solve (3.29). Now if we look at the driving terms in (3.29) along with the definitions of the L's, we see that there are two types; (a) those proportional to N, and (b) those proportional to N^2. The former are nothing but higher-order corrections to the Born-approximation for the scattering of an electron on a single scattering center. The latter are connected with the interference between the scattering from two centers, and we shall refer to them as the "multiple scattering terms." We write

$$f_l{}^{(21)}=f_l{}^{(a)}+f_l{}^{(b)} \tag{4.22}$$

to express this decomposition, and write the corresponding velocity contributions as $v_\beta{}^{(a)}$ and $v_\beta{}^{(b)}$. The calculation of $v_\beta{}^{(a)}$ is rather tedious, even with all the

simplifications used in this section, and we shall not give it here. In any case, it is not of any great interest since it represents only a correction (in the sense of perturbation theory in λ) to $v_\beta^{(11)}$. It will have, in general, the order of magnitude

$$v_\beta^{(a)} \sim \lambda v_\beta^{(11)}. \tag{4.23}$$

The quantity $f_l^{(b)}$ represents, on the other hand, a new physical effect. In the equation for $f_l^{(b)}$, of all the driving terms only that part of (3.31) proportional to N contributes. Let us call the corresponding part of $L_{ll'}^{(21)}$, $B_{ll'}$. Then the spin-orbit part of $B_{ll'}$, in the limit we are considering, becomes

$$B_{ll'}=\frac{(2\pi)^2 n^2 \bar{\varphi}^4}{2i\Omega^2}\delta(\omega_{ll'})\sum_{l'',l'''}\delta(\omega_{ll''})P\left(\frac{1}{\omega_{ll'''}}\right)(k\times k'+k'\times k''+k''\times k)_{\mu\nu}$$
$$\times\left\{\delta_{nn'}\delta_{n'n''}\delta_{n''n'''}\left(\frac{\partial J_\nu{}^l}{\partial k_\mu}-\frac{\partial J_\mu{}^l}{\partial k_\nu}\right)_0+\tfrac{1}{2}\delta_{nn'}\delta_{n'n''}(J_\mu{}^{nn'''}(k)J_\nu{}^{n'''n}(k)-J_\nu{}^{nn'''}(k)J_\mu{}^{n'''n}(k))\right\}$$
$$\times(\delta_{k-k'+k''-k''',0}+\delta_{k-k'-k''+k''',0}+\delta_{k+k'-k''-k''',0}), \tag{4.24}$$

where

$$(k\times k')_{\mu\nu}=k_\mu k_\nu'-k_\nu k_\mu'. \tag{4.25}$$

Carrying out the l'' and the l''' summations yields

$$B_{ll'}=\frac{\pi i n^2\bar{\varphi}^2}{\Omega I_0}\delta(\omega_{ll'})(k\times k')_{\mu\nu}$$
$$\times\left\{\frac{3}{2}T_{\mu\nu}^{(0)}-(2m^*)S\left(\frac{\partial J_\nu{}^l}{\partial k_\mu}-\frac{\partial J_\mu{}^l}{\partial k_\nu}\right)_0\right\}, \tag{4.26}$$

with

$$T_{\mu\nu}^{(0)}=\sum_{l'''}{}'\left(\frac{J_\mu{}^{ll'''}J_\nu{}^{l'''l}-J_\nu{}^{ll'''}J_\mu{}^{l'''l}}{\omega_{ll'''}}\right)_{k=0} \tag{4.27}$$

and

$$S=\frac{1}{2k|k-k'|}\log\left(\frac{2k+|k-k'|}{2k-|k-k'|}\right)+\frac{1}{|k+k'|^2}. \tag{4.28}$$

Calculating the resultant average velocity from this by the method followed in all previous cases, we obtain

$$v_\beta^{(b)}=ieE_\alpha\left[\left(\frac{\partial J_\beta{}^l}{\partial k_\alpha}-\frac{\partial J_\alpha{}^l}{\partial k_\beta}\right)C-\epsilon_F T_{\alpha\beta}^{(0)}\right]. \tag{4.29}$$

The quantity C is a numerical constant,

$$C=(17/30)+(8/15)\ln 2\cong 0.94. \tag{4.30}$$

5. DISCUSSION OF RESULTS

Our final result for the extra current due to spin-orbit coupling consists of three parts: (1) $v_\beta^{(11)}$, from (4.17); (2) u_β, from (4.21); and (3) $v_\beta^{(b)}$, from (4.29). The first of these is included in conventional transport theory, and was considered (from a somewhat different point of view) by Smit and by Luttinger.[8] Since it is proportional to $1/n$ it gives rise to an anomalous Hall coefficient (R') which is proportional to n. If the resistivity of the sample is varied by varying the impurity content, then this will give rise to an R' which is proportional to the resistivity of the sample. For this reason, such a term does not seem to the author to be able to explain the experimental data. For iron, for example, the experimental results of Kooi[9] show a dependence on the square of the resistivity (to a good approximation). This same resistivity dependence is true to all orders of Born approximation in the conventional transport theory, and therefore if something else is needed one must go beyond the framework of this theory.

The contribution (2) was first considered by Karplus and Luttinger. By a very crude approximation, they attempted to take into account more than just the diagonal elements of the density matrix and velocity operator, as is done in conventional theory. The result was of the same general order of magnitude as (4.21). This term, being independent of n does give an R' proportional to the square of the resistivity as desired. If we compare (1) and (2), we see that in our approximation their relative values are

$$v_\beta^{(11)}/u_\beta=\epsilon_F/(3n\bar{\varphi}). \tag{5.1}$$

Therefore at extremely low density of impurities, the ordinary scattering term $v_\beta^{(11)}$ must dominate, and one should see an R' proportional to the resistivity. Finally, however, as the density of impurities increases we must go over to a resistivity-squared domain. Whether this is already true for Si in Fe at the densities used by Kooi, for example, is open to some question, but it is certainly not excluded by an estimate of the type (5.1).

It should also be mentioned perhaps that the terms previously found by Karplus and Luttinger correspond to the first term of (3.6) and the last term of (3.15). It is possible to write the formulas in such a way that these terms are exactly canceled by some of the terms which originally depended explicitly on the scattering potential. This decomposition [which is used to establish (3.26)] seems to us to have no particular physical significance, since when it is performed the remaining objects (g_l and $w_\alpha{}^l$) are no longer phase-invariant. (That is, they change their values if the

[8] J. M. Luttinger, Berkeley, 1953 (unpublished).

[9] C. Kooi, Phys. Rev. **95**, 843 (1954).

phase of the original set of Bloch functions are changed.) The total result u_β is, of course, still phase-invariant. In any case, the important result from our point of view is that no matter how one chooses to interpret the different pieces which make up u_β, its final order of magnitude is roughly that given by Karplus and Luttinger.

The final term (3), which results from multiple-scattering corrections to the transport equation, is new. The first term of (4.29) is exactly of the same form as u_β, and in fact cancels out a good part of it. It is doubtful if this approximate cancellation holds in anything but the extreme effective-mass limit, since very different quantities actually enter into $v_\beta^{(b)}$ and u_β. It seems more reasonable to conclude simply that the multiple scattering term will in general give a contribution comparable in order of magnitude with the off-diagonal and field corrections, and that to take one without the other is inconsistent. The last term of (4.29) is, from (B.23), of the order of magnitude of ϵ_F/Δ (where Δ is a typical separation energy between the $k=0$ edges of two bands). We should really drop such a term to be consistent with our extreme effective-mass limit. We leave it in, however, to indicate that other types of terms besides $(\partial J_\beta{}^l/\partial k_\alpha - \partial J_\alpha{}^l/\partial k_\beta)_0$ can occur. For a realistic case, of course, ϵ_F will be of the same order of magnitude as Δ, and this type of term will contribute significantly.

APPENDIX A. DISCUSSION OF SOME COMMENTS OF J. SMIT

In several interesting papers, Smit[10] has criticized the results of Karplus and Luttinger, and has also questioned in general the occurrence of contributions to the average velocity from off-diagonal components of the density matrix. While we cannot claim to understand many of Smit's points, he is without doubt correct in regarding the results of Karplus and Luttinger as representing a considerable oversimplification of the situation. We can indicate rather precisely just how this comes about from the point of view of our present formalism, and shall do this below. We wish to stress, however, that although the treatment of Karplus and Luttinger was not complete, the present calculation shows that the effect does exist and is of the same order of magnitude. Smit's second point (the noncontribution of off-diagonal matrix elements) seems less correct to us, and we also wish to discuss it briefly.

We can connect the work of Karplus and Luttinger with this paper in the following manner. The matrix elements of the electric field perturbation H are given by

$$H_1 = H_a + H'', \tag{A.1}$$

where

$$H_a = -ieE_\alpha \delta_{nn'}(\partial\delta_{kk'}/\partial k_\alpha), \tag{A.2}$$

$$H'' = -ieE_\alpha J_\alpha{}^{ll'}. \tag{A.3}$$

[10] J. Smit, Physica **21**, 877 (1955); Physica **24**, 39 (1958).

The idea of Karplus and Luttinger was to include H'' in the unperturbed Hamiltonian, since it is perfectly regular and has the same translational symmetry as H_0. Now if we write the field-dependent part of the density matrix (f) in the form

$$f = \tilde{f} + \rho(H+H'') - \rho(H), \tag{A.4}$$

it is easy to see that $\tilde{f}$ satisfies (to the first order in E_α) the equation

$$[H,\tilde{f}] - is\tilde{f} = \tilde{C}, \tag{A.5}$$

$$\tilde{C} = (\rho(H), H_a). \tag{A.6}$$

f satisfies the same equation except that $\tilde{C}$ is replaced by C; therefore, we have completely eliminated H'', and its only effect is to replace $\rho(H)$ by $\rho(H+H'')$ as the "unperturbed density" matrix. The average velocity is given by

$$\bar{v}_\beta = \tilde{v}_\beta + \tilde{u}_\beta, \tag{A.7}$$

$$\tilde{v}_\beta = \mathrm{tr}(\tilde{f}v_\beta), \tag{A.8}$$

$$\tilde{u}_\beta = \mathrm{tr}[(\rho(H+H'') - \rho(H))v_\beta]. \tag{A.9}$$

To the lowest order in λ we can compute $\tilde{u}_\beta$ at once, by going over to the representation which makes H_0+H'' diagonal. This gives

$$\tilde{u}_\beta{}^{(0)} = ieE_\alpha \sum_l \rho_l \left(\frac{\partial J_\beta{}^l}{\partial k_\alpha} - \frac{\partial J_\alpha{}^l}{\partial k_\beta} \right) + ieE_\alpha \sum_l \rho_l \frac{\partial J_\alpha{}^l}{\partial k_\beta}, \tag{A.10}$$

which is exactly the result of Karplus and Luttinger. Now since

$$\tilde{C}_{ll'} = ieE_\alpha \left(\frac{\partial}{\partial k_\alpha} + \frac{\partial}{\partial k_\alpha'} \right) \rho_{ll'}, \tag{A.11}$$

Eq. (A.5) no longer contains the J matrix explicitly and is very much like corresponding equation with no periodic potential. Karplus and Luttinger's approximation consists in just replacing this equation by the equation of ordinary transport theory, that being all that was known at the time. Then there is no contribution to the Hall effect from $\tilde{f}$ and we get (A.10) as our final result. That (A.10), however, cannot be the whole story follows at once from the fact that it is not invariant under a change in phase of the Bloch functions. Various arguments were given at the time to justify this, but we no longer regard them as convincing and shall not repeat them here. The point is that since $\tilde{u}_\beta{}^{(0)}$ is of order λ^0, we cannot throw away the corrections to $\tilde{f}$ of order λ^0, which corrections go beyond the usual transport theory. Taking them into account leads at once to the formulas of the text.

We now come to Smit's second point. Let us first consider an electron in a pure state ψ, under the simultaneous influence of an electric field and collisions. Expand ψ in Bloch waves,

$$\psi = \sum a_l(t)\psi_l. \tag{A.12}$$

Smit first considers the average *position* $\bar{x}_\alpha$ of the electron. This is given by

$$\bar{x}_\beta = i\sum_l \frac{\partial a_l}{\partial k_\beta} a_l^* + i\sum_{l,l'} a_{l'} a_l^* J_\beta^{ll'}. \tag{A.13}$$

If we average over an ensemble of electrons and call the average value of $a_{l'}a_l^*$ the density matrix $(\rho_T)_{l'l}$, then

$$\bar{x}_\beta = i\sum_l \left[\frac{\partial(\rho_T)_{nk,\,nk'}}{\partial k_\beta}\right]_{k'=k} + i\sum_{l,l'} (\rho_T)_{l'l} J_\beta^{ll'}. \tag{A.14}$$

Smit argues that the last term of (A.14) cannot contribute to the average velocity (defined as the time derivative of $\bar{x}_\beta$). This is certainly true. In our formalism we have

$$\rho_T = \rho + fe^{st}, \tag{A.15}$$

$$\dot{\rho}_T = sfe^{st} = sf, \tag{A.16}$$

at $t=0$. Therefore the last term gives a velocity contribution proportional to s, which vanishes in the limit $s \to 0$. Therefore, in agreement with Smit, we may write

$$\bar{v}_\beta = \dot{\bar{x}}_\beta = i\sum_l \left[\frac{\partial(\dot{\rho}_T)_{nk,\,nk'}}{\partial k_\beta}\right]_{k'=k}. \tag{A.17}$$

Smit interprets (A.17) as meaning that there is no off-diagonal ($n \neq n'$) contribution to $\bar{v}_\beta$. We cannot agree with this interpretation. First of all, if we replace $i\dot{\rho}_T$ in (A.17) by its value $[H_T,\rho_T]$, then we obtain at once the formulas of the text, including off-diagonal elements. On the other hand, if we use (A.16) we obtain

$$\bar{v}_\beta = is\sum_l \left(\frac{\partial f_{nk,\,nk'}}{\partial k_\beta}\right)_{k'=k}. \tag{A.18}$$

Since $\bar{v}_\beta$ is finite as $s \to 0$, the quantity in brackets must have a $1/s$ singularity, and its calculation goes beyond the ordinary transport theory which computes only f_l, or KLI which computes the f itself (which is regular in the limit $s \to 0$). The great advantage in using the velocity operator $v_\beta = i[H_T,x_\beta]$ is that it enables us to avoid such difficult expressions as occur in (A.18).

Smit tries to go a little further with (A.17) itself. He puts $(\rho_T)_{ll'} = a_l a_{l'}^*$ (as is true for a pure state). Then, since the diagonal values of ρ_T approach constants (those of $\rho+f$), he puts

$$a_l = |a_l| e^{-iE_l t}, \tag{A.19}$$

where $|a_l|$ is constant, and E_α has the dimensions of an energy. This gives for $\bar{v}_\beta$

$$\bar{v}_\beta = \sum_l (\rho_T)_{ll} \frac{\partial E_l}{\partial k_\beta}, \tag{A.20}$$

which is really of the form of a sum over diagonal elements of the density matrix. This result seems to us to be erroneous. First of all, we are *not* describing a pure state, and therefore the representation $a_l a_{l'}^*$ of the density matrix does not exist. Second, this representation actually leads to a contradiction since if it were true the off-diagonal elements of ρ_T would oscillate with frequency $E_l - E_{l'}$, and therefore have an average value zero. On the other hand, from KLI we know that such elements exist in general (they are just those of $\rho+f$).

It is, incidentally, always possible to write the average value of any operator in terms of a sum over the diagonal matrix elements of f_l, since it is characteristic of our theory that the off-diagonal matrix elements may always be expressed in terms of the diagonal ones. The resulting "effective velocity operator," however, is not, in general, of the form $\partial E_l/\partial k_\beta$, as may be easily seen from the explicit expressions of this paper.

APPENDIX B. REALITY PROPERTIES

In this section some of the reality properties of the matrix elements occurring in the theory will be derived. Most of these were already given in the paper of Karplus and Luttinger, but there they are so seriously marred by numerous misprints that we prefer to give them here again. The derivation is rather simpler also.

We consider first the case of an electron in a periodic potential with no spin-orbit coupling. The Hamiltonian will be written H_{00},

$$H_{00} = p^2/2m + U, \tag{B.1}$$

and the eigenfunctions are

$$\phi_l = (e^{ik\cdot r}/\sqrt{\Omega}) u_l(r). \tag{B.2}$$

As usual, l stands for the index pair (n,k), and u_l is the periodic part of the Bloch function.

We shall assume that the crystal has a center of symmetry, so that $U(r) = U(-r)$. Further, H_{00} is real (which is equivalent to time inversion symmetry for our problem). Therefore, under the symmetry operation (S) which replaces r by $-r$ and takes the complex conjugate, the Hamiltonian is invariant and

$$SH_{00}S^{-1} = H_{00}. \tag{B.3}$$

Under this transformation the function ϕ_l becomes

$$\phi_l' = S\phi_l = \phi_{n,k}^*(-r). \tag{B.4}$$

Therefore, since S commutes with H_{00}, we can choose the ϕ_l to be eigenfunctions of S also. That is,

$$S\phi_l = S'\phi_l. \tag{B.5}$$

However, S^2 is again the identity operation and therefore the eigenvalues S' must satisfy $S'^2 = 1$ or $S' = \pm 1$. The ϕ_l and ϵ_l are however continuous functions of k, and therefore as we vary k in a band S' cannot

change sign suddenly. It follows then that

$$S\phi_l=\phi_{nk}^*(-\mathbf{r})=\delta_n\phi_{nk}(\mathbf{r}), \tag{B.6}$$

where $\delta_n=\pm 1$, depending on the band in question.

For any Hermitian operator A which is invariant under S, the matrix elements satisfy the following reality condition:

$$\begin{aligned}(\phi_l,A\phi_{l'})^*&=\left(\int\phi_l^*(\mathbf{r})A\phi_l(\mathbf{r})d\mathbf{r}\right)^*\\&=\int\phi_l(\mathbf{r})A^*\phi_{l'}^*(\mathbf{r})d\mathbf{r}\\&=\delta_n\delta_{n'}\int\phi_l^*(-\mathbf{r})A^*\phi_{l'}(-\mathbf{r})d\mathbf{r}\quad[\text{by (B.6)}]\\&=\delta_n\delta_{n'}\int\phi_l^*(\mathbf{r})A^*(-\mathbf{r})\phi_{l'}(\mathbf{r})d\mathbf{r}\\&=\delta_n\delta_{n'}\int\phi_l^*(\mathbf{r})A(\mathbf{r})\phi_{l'}(\mathbf{r})d\mathbf{r}\\(\phi_l,A\phi_{l'})^*&=\delta_n\delta_{n'}(\phi_l,A\phi_{l'}).\end{aligned} \tag{B.7}$$

For any Hermitian operator B which changes sign under S (for example, the spin-orbit coupling), the identical method of proof gives

$$(\phi_l,B\phi_{l'})^*=-\delta_n\delta_{n'}(\phi_l,B\phi_{l'}). \tag{B.8}$$

This equation means, in particular, that the diagonal elements of any such operator vanish identically, since by the Hermiticity they are real and by (B.8) they are pure imaginary. (Therefore, there are no first order corrections to the energy due to spin-orbit coupling, and we make no distinction between $\epsilon_l^{(0)}$ and ϵ_l.)

If there is spin-orbit coupling present, the Hamiltonian is H_0 defined by (2.13), with the eigenfunctions and values given by (2.18) and (2.19). The spin-orbit coupling,

$$H^{\text{s.o.}}=(\mathbf{q}\times\nabla U)\cdot\mathbf{p}, \tag{B.9}$$

is an operator of type B. We shall limit ourselves to effects of (B.9) to the first order. Then

$$\psi_l=\phi_l+\phi_l^{(1)}, \tag{B.10}$$

where $\phi_l^{(1)}$ is of the first order in $H^{\text{s.o.}}$. It follows at once that $\phi_l^{(1)}$ must satisfy

$$(\phi_l^{(1)}(-\mathbf{r}))^*=-\delta_n\phi_l^{(1)}(\mathbf{r}), \tag{B.11}$$

instead of (B.6). If we have any operator D, we will write its matrix elements

$$D_{ll'}\equiv(\psi_l,D\psi_{l'})=D_{ll'}{}^{(0)}+D_{ll'}{}^{(1)}, \tag{B.12}$$

where the $D_{ll'}{}^{(0)}$ are the matrix elements of the operator in the representation without spin-orbit coupling, and $D_{ll'}{}^{(1)}$ are the corrections to the first order due to spin-orbit coupling. Then from (B.11) it follows at once that

$$\begin{aligned}A_{ll'}{}^{(1)*}&=-\delta_n\delta_{n'}A_{ll'}{}^{(1)},\\B_{ll'}{}^{(1)*}&=+\delta_n\delta_{n'}B_{ll'}{}^{(1)}.\end{aligned} \tag{B.13}$$

Finally we consider the reality properties of the quantities $J_\alpha{}^{ll'}$ defined by (2.17). From the orthonormality of the ψ_l we have at once

$$J_\alpha{}^{ll'}+(J_\alpha{}^{l'l})^*=0. \tag{B.14}$$

We write

$$J_\alpha{}^{ll'}=I_\alpha{}^{ll'}+K_\alpha{}^{ll'}, \tag{B.15}$$

where I is the contribution of zeroth order in the spin-orbit coupling, and K is the contribution of the first order. From (2.17) we have

$$\begin{aligned}(I_\alpha{}^{ll'})^*&=\frac{\delta_{kk'}}{\omega_c}\int_{\omega_c}u_l\frac{\partial u_{l'}^*}{\partial k_\alpha'}d\mathbf{r}=\frac{\delta_{kk'}}{\omega_c}\int u_l(-\mathbf{r})\frac{\partial u_{l'}^*(-\mathbf{r})}{\partial k_\alpha'}d\mathbf{r}\\&=\frac{\delta_{kk'}}{\omega_c}\left[\int u_l^*(\mathbf{r})\frac{\partial u_{l'}(\mathbf{r})}{\partial k_l'}\right]\delta_n\delta_{n'}=\delta_n\delta_{n'}I_\alpha{}^{ll'},\end{aligned} \tag{B.16}$$

and similarly

$$(K_\alpha{}^{ll'})^*=-\delta_n\delta_{n'}(K_\alpha{}^{ll'}). \tag{B.17}$$

From (B.14) we have that the diagonal elements of J satisfy

$$(J_\alpha{}^l)^*=-J_\alpha{}^l, \tag{B.18}$$

so that they are pure imaginary. Therefore from (B.16) we find

$$I_\alpha{}^l=0, \tag{B.19}$$

with our choice for the phases of the Bloch functions. $K_\alpha{}^l$ on the other hand is not zero in general, so that the diagonal elements of J are proportional to the spin-orbit coupling.

We also list here certain other properties of the J operators which are convenient in our work. For any operator Λ we have

$$(\Lambda,x_\alpha)_{ll'}=\frac{1}{i}[D_\alpha\Lambda_{ll'}+(J_\alpha,\Lambda)_{ll'}], \tag{B.20}$$

where

$$D_\alpha=\partial/\partial k_\alpha+\partial/\partial k_\alpha'. \tag{B.21}$$

If $\Lambda=Q$, a function of position alone, then

$$(Q,J_\alpha)_{ll'}=D_\alpha Q_{ll'}. \tag{B.22}$$

Finally

$$\begin{aligned}(J_\alpha,J_\beta)_{ll'}&=\sum_{l''}(J_\alpha{}^{ll''}J_\beta{}^{l''l'}-J_\beta{}^{ll''}J_\alpha{}^{l''l'})\\&=\left[\frac{\partial J_\alpha{}^{nn'}(k)}{\partial k_\beta}-\frac{\partial J_\beta{}^{nn'}(k)}{\partial k_\alpha}\right]\delta_{kk'},\end{aligned} \tag{B.23}$$

where

$$J_\alpha^{nn'}(k)=\frac{1}{\omega_c}\int_c w_{nk}^*\frac{\partial w_{n'k}}{\partial k_\alpha}dr. \quad \text{(B.24)}$$

APPENDIX C. EFFECTIVE-MASS APPROXIMATION TO MATRIX ELEMENTS $\varphi_{ll'}$

The matrix elements $\varphi_{ll'}$ are given by (2.25) or

$$\varphi_{ll'}=\frac{1}{\Omega}\int e^{-i(k-k')\cdot r}\varphi w_l^* w_{l'}dr. \quad \text{(C.1)}$$

The assumption that φ has no Fourier components of the order of a reciprocal lattice vector means that only the constant part of the periodic function $w_l^* w_{l'}$ can contribute. Therefore

$$\varphi_{ll'}=\varphi_{kk'}W_{ll'}, \quad \text{(C.2)}$$

where

$$\varphi_{kk'}=\frac{1}{\Omega}\int e^{-i(k-k')\cdot r}\varphi dr, \quad \text{(C.3)}$$

$$W_{ll'}=\frac{1}{\omega_c}\int_{\omega_c} w_l^* w_{l'}dr. \quad \text{(C.4)}$$

The quantity $\phi_{kk'}$ is just the plane-wave matrix element of the potential. Since the latter is assumed to have no Fourier components of the order of a reciprocal lattice vector, k' must be close to k and we may expand $W_{ll'}$ as

$$W_{ll'}=\frac{1}{\omega_c}\int w_{nk}^*\left[w_{n'k}+(k_\mu'-k_\mu)\frac{\partial w_{n'k}}{\partial k_\mu}+\cdots\right]dr$$
$$=\delta_{nn'}+(k_\mu'-k_\mu)J_\mu^{nn'}(k)+\tfrac{1}{2}(k_\mu'-k_\mu)(k_\nu'-k_\nu)\times J_{\mu\nu}^{nn'}(k)+\cdots, \quad \text{(C.5)}$$

where $J_\alpha^{nn'}(k)$ is given by (B.24) and

$$J_{\mu\nu}^{nn'}(k)=\frac{1}{\omega_c}\int_{\omega_c} w_{nk}^*\frac{\partial^2 w_{n'k}}{\partial k_\mu \partial k_\nu}dr. \quad \text{(C.6)}$$

The $J_{\mu\nu}^{nn'}(k)$ satisfy the identity

$$J_{\mu\nu}^{nn'}(k)-(J_{\mu\nu}^{n'n}(k))^*=\frac{\partial J_\mu^{nn'}(k)}{\partial k_\nu}+\frac{\partial J_\nu^{nn'}(k)}{\partial k_\mu}, \quad \text{(C.7)}$$

which follows at once the orthonormality of the w_l's.

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Magnetic Structure of Fe_4N†

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The magnetic structure of Fe_4N has been examined in a neutron diffraction study. The results are in agreement with a model proposed by Wiener and Berger on the basis of magnetic measurements on a series of related compounds. Ferromagnetically aligned moments of 3 μ_B and 2 μ_B are found for the corner and face-center Fe atoms (respectively) in the cubic unit cell. The difference in moments is apparently due to bonding interaction between nitrogen, at the body-center position, and the face-center Fe's.

INTRODUCTION

THE nitride Fe_4N is a magnetic compound with a Curie point at 488°C and a net moment per formula unit of about 9 Bohr magnetons (extrapolated measurement: 8.86 μ_B at 0°K).[1] The average moment per iron atom is thus almost identical with that observed in body-centered α-iron (2.22 μ_B). The crystal structure is most closely related to nonmagnetic face-centered γ-iron, however. It may be considered as simply an expanded γ-iron lattice with nitrogen placed at the body-center of the unit cell.[2] The magnetic

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