Quantum theory of Ohmic galvano- and thermomagnetic effects in semiconductors*

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A density-matrix formalism developed earlier for the evaluation of Ohmic magnetoconductivity is further elaborated and applied to other magnetotransport effects in nonpolar semiconductors in the presence of a magnetic field of arbitrary strength. The difference from earlier transport theories lies in a natural extension of the scattering dynamics beyond the strict Born approximation. The well-known divergence difficulties of older theories, usually removed by any of a number of *ad hoc* cutoff procedures, do not appear here. The transverse-conductivity expression turns out to be equivalent to that of some earlier theories of cyclotron resonance extrapolated to zero frequency, but derived in a different way. When applied to elastic scattering of electrons in a simple model of a semiconductor, the theory gives galvanomagnetic and thermomagnetic coefficients within the range of values usually seen experimentally, showing the basic correctness of the theory. It is then applied to the magnetophonon effect, where the resonance peaks are shown to be finite. An interesting inversion of one of the peaks in the Ettingshausen-Nernst coefficient is found. Landau-level broadening and phonon drag are not included in the present paper, although they can be incorporated when deemed important.

I. INTRODUCTION

We present in this paper a first-principles theory for the calculation of galvanomagnetic and thermomagnetic effects, in the framework of a density-matrix formalism given earlier.[1] In order to bring out the essential points of the theory, we develop it for electrons in the parabolic bands of nondegenerate, nonpolar semiconductors, not including this time phonon drag, anisotropy of the energy surface, and multiple valleys.[1] The theory is illustrated by applying it to the magnetophonon effect[2] as well as to elastic scattering of electrons by acoustic phonons.

Transverse and longitudinal magnetoresistance are two of the most investigated properties of semiconductors. Although the theories for the longitudinal case based on the solution of the Boltzmann transport equation have been reasonably successful,[2-6] the transverse case appears to be elusive, as can be seen from the conflicting results obtained by many authors.[7-12] In this case, the component of the path of the electron in the direction of current flow is strongly affected by the magnetic field. For low magnetic fields, this effect may be considered as a perturbation with a relaxation time approximated by its zero-field value in the Boltzmann transport equation. The earlier theories based on this approximation[3,13,14] predicted a saturation in the transverse magnetoresistance. As we now know from many experimental results (examples are found in Refs. 2 and 15–17), there is no such saturation; rather the magnetoresistance increases almost linearly with increasing magnetic field. The effect of quantization of the electronic energy levels on the relaxation time removes the saturation.

The curvature in the free path of electrons between two scattering centers introduces nondiagonal elements of the velocity operator in the transverse case. Therefore, off-diagonal elements of the density matrix are needed to determine the ensemble average of the current. On the other hand, for the longitudinal configuration in a parabolic-band semiconductor, the velocity operator is diagonal and hence the Boltzmann transport equation can be used. For an anisotropic energy surface, exemplified by n-germanium, even for the longitudinal case some anisotropic effects[1] occur which cannot be described by the Boltzmann equation,[18] and a density-matrix approach is required. Critiques of the Boltzmann equation and discussions of the importance of the density matrix in transport problems are given in many papers, e.g., Refs. 6, 7, 19, and 20.

The best-known recent theories of transverse magnetoresistance based on a density-matrix approach still have the unpleasant drawback of divergences,[9] necessitating the introduction of some kind of cutoff mechanism to achieve finite results.[9,21] The results are clearly very sensitive to the cutoff assumed. These theories are essentially expansions in powers of $(\omega_c\tau)^{-1}$ with only the first-order term retained. Here, ω_c is the cyclotron frequency and τ is an average momentum relaxation time. The divergence difficulties arise because the electrons making transitions to the bottoms of the Landau subbands have relaxation times which are very small, thus violating the condition $\omega_c\tau \gg 1$ upon which the theories are based.

The theory presented here is not a strict Born-approximation theory, and is not restricted to $\omega_c\tau \gg 1$. In fact, it is finite for $1/\tau \to \infty$, and correctly reduces to the zero-field theory as $B \to 0$. The expressions for the transport coefficients have the so-called "classical cutoff" form[9]; this, however, is not an *ad hoc* insertion, but a natural consequence of the theory. Another consideration sometimes used as a cutoff procedure in previous theories, that of taking the acoustic-phonon scattering to be inelastic, is unimportant in the present theory. Likewise, broadening of the Landau levels through collisions is not responsible for the finiteness of the theory. Level broadening can be inserted just as in the earlier theories when deemed important, e.g., in analyses of resonance amplitudes.[22] Phonon drag or disturbance of the phonon distribution can be important in the crossed-field configuration as shown earlier,[1] but is not taken into account in the present paper.

In spite of a large amount of experimental and theoretical work in magnetoresistance, there have been relatively few attempts to compare the theoretical results in detail with existing experimental data. For thermomagnetic effects, the amount of work done is relatively smaller than for the galvanomagnetic effects. The derivative techniques which have been so successful in measurements of oscillatory galvanomagnetic effects[2] have not yet been exploited fully to study these interesting effects in thermomagnetism. There have been only a few theoretical calculations to interpret the experimental data. We hope that the present paper and its predecessor[1] will encourage many to attempt to correlate both galvano- and thermomagnetic data with the type of theory given here.

In Sec. II, the steady-state density matrix for the electron system is derived, assuming the phonon distribution to be in equilibrium, and treating the electric field as a perturbation. With this density matrix, the electric and energy currents are derived in Sec. III, from which the magnetotransport coefficients are obtained. The application of the theory to elastic scattering and to magnetophonon structure by presentation and discussion of numerical results is the subject of Sec. IV, where a few concluding remarks are also given.

II. BASIC FORMALISM

The Hamiltonian for a coupled electron-phonon system having a parabolic conduction band characterized by an isotropic effective mass m^* and an electron charge $-e$ may be written

$$H_T = H_0 + H \,, \tag{2.1}$$

where the unperturbed part H_0 is the sum of electron and lattice Hamiltonians, H_e and H_L, given by

$$H_e = [\, p_x^2 + p_z^2 + (p_y + m^*\omega_c x)^2]/2m^* \,, \tag{2.2}$$

$$H_L = \sum \hbar\omega_{qi}(N_{qi} + \tfrac{1}{2}) \,, \tag{2.3}$$

where

$$\omega_c = eB/m^* \,. \tag{2.4}$$

The magnetic field $\vec{B}$ is in the z direction, and the usual Landau gauge is used in Eq. (2.2). The summation in the lattice Hamiltonian is over all phonon wave vectors $\vec{q}$ in each branch i (which are the longitudinal optic and acoustic branches in the present paper); N_{qi} and ω_{qi} are, respectively, the number operator and frequency of these phonons. The perturbation H in our treatment is

$$H = \sum_i V_i + e\vec{E}\cdot\vec{r} \,, \tag{2.5}$$

where V_i is the electron-lattice deformation potential interaction for branch i phonons[23]:

$$V_i = iE_i \sum_q \left(\frac{\hbar\omega_{qi}}{2\Omega\rho_d u_l^2}\right)^{1/2} b_{qi}\, e^{i\vec{q}\cdot\vec{r}} + \text{H.c.} \tag{2.6}$$

Here $\vec{r}$ is the electron position operator, ρ_d is the crystal density, Ω is its volume, u_l is the average longitudinal sound velocity, b_{qi} is the phonon destruction operator, and E_i is the deformation potential energy corresponding to optic or acoustic phonons.

The term $e\vec{E}\cdot\vec{r}$ describes the interaction of the electron with the external electric field $\vec{E}$, and is included in the perturbation H since this ensures the homogeneous distribution of the electrons[1] in the absence of the perturbation.

The eigenvalues of H_e are

$$\epsilon_{nk} = (n + \tfrac{1}{2})\hbar\omega_c + \hbar^2 k_z^2/2m^*, \qquad n = 0, 1, 2, \ldots \tag{2.7}$$

corresponding to electron wave functions which are products of plane-wave states in the y and z directions, and harmonic oscillator functions for the quantized orbital motion.[9] In Eq. (2.7) and hereafter, the single index k will be used to denote the pair of electron wave numbers k_y and k_z. In the Appendix we give several matrix elements and relationships used in the calculations.

The eigenvalues of H_L are given simply by replacing the N_{qi} in Eq. (2.3) by the phonon quantum numbers $n_{qi} = 0, 1, 2, \ldots$.

The physical quantities of interest here are the electric and energy currents, which are found by use of a steady-state density matrix. The complete density matrix $\rho_T(t)$ is the solution to the quantum-mechanical Liouville equation

$$\frac{d\rho_T(t)}{dt} = \frac{i}{\hbar}[\,\rho_T(t),\, H_T(t)] \,. \tag{2.8}$$

Using a common procedure,[19] we assume that the perturbation is turned on adiabatically at $t = -\infty$,

so that

$$H_T(t) = H_0 + He^{\eta t} , \tag{2.9}$$

where η is a positive number much smaller than any of the relaxation rates of the system, and eventually taken to be vanishingly small. The density matrix should then follow a similar time behavior:

$$\rho_T(t) = \rho^0(H_0) + \rho e^{\eta t} . \tag{2.10}$$

The initial equilibrium density matrix $\rho^0(H_0)$ factors into electron and lattice parts

$$\rho^0(H_0) = f^0(H_e)\rho_L(H_L) , \tag{2.11}$$

diagonal in the H_e and H_L eigenfunctions. The diagonal elements of $f^0(H_e)$ form the Fermi-Dirac distribution function, which reduces to the Maxwell-Boltzmann distribution for our case of a nondegenerate semiconductor:

$$f^0_{nk} \equiv \langle nk | f^0 | nk \rangle = [e^{\beta(\epsilon_{nk}-\xi)} + 1]^{-1}$$

$$\approx e^{\beta\xi} e^{-\beta\epsilon_{nk}}$$

$$= n_e(2\pi\hbar^2\beta/m^*)^{3/2}[\sinh(\tfrac{1}{2}s)/s]\, e^{-\beta\epsilon_{nk}} , \tag{2.12}$$

where $\beta = 1/k_B T$, n_e is the electron concentration, and

$$s = \beta\hbar\omega_c . \tag{2.13}$$

Similarly, the matrix elements of $\rho_L(H_L)$ are proportional to $\exp[-E_L(\{n_q\})]$, where $\{n_q\}$ represents the set of all phonon quantum numbers. The ensemble average of N_{qi} with respect to $\rho_L(H_L)$ is the number of thermal phonons of type $\vec{q}, i$:

$$\langle n_{qi} \rangle = (e^{\beta\hbar\omega_{qi}} - 1)^{-1} . \tag{2.14}$$

Now we proceed to establish the form of the steady-state density matrix ρ. Denoting the set of quantum numbers n, k_y, k_z, $\{n_q\}$ by α, and using subscripts to denote matrix elements, one finds from Eqs. (2.8)–(2.10) at $t = 0$

$$S_{\alpha\alpha'}\rho_{\alpha\alpha'} = P_{\alpha\alpha'} + [\rho, H]_{\alpha\alpha'} , \tag{2.15}$$

where

$$S_{\alpha\alpha'} = E_{\alpha\alpha'} - i\hbar\eta , \tag{2.16}$$

$$E_{\alpha\alpha'} = E_\alpha - E_{\alpha'} , \tag{2.17}$$

$$P_{\alpha\alpha'} = [\rho^0, H]_{\alpha\alpha'} . \tag{2.18}$$

Dividing Eq. (2.15) by $S_{\alpha\alpha'}$ and replacing ρ on the right side by the resultant expression, one gets

$$S_{\alpha\alpha'}\rho_{\alpha\alpha'} = P_{\alpha\alpha'} + P'_{\alpha\alpha'} + P''_{\alpha\alpha'} , \tag{2.19}$$

where

$$P'_{\alpha\alpha'} = \sum_{\alpha_1} (S^{-1}_{\alpha\alpha_1} P_{\alpha\alpha_1} H_{\alpha_1\alpha'} - H_{\alpha\alpha_1} S^{-1}_{\alpha_1\alpha'} P_{\alpha_1\alpha'}) \tag{2.20}$$

and

$$P''_{\alpha\alpha'} = \sum_{\alpha_1, \alpha_2} (S^{-1}_{\alpha\alpha_1}\rho_{\alpha\alpha_2} H_{\alpha_2\alpha_1} H_{\alpha_1\alpha'} + S^{-1}_{\alpha_1\alpha'} H_{\alpha\alpha_1} H_{\alpha_1\alpha_2}\rho_{\alpha_2\alpha'} - S^{-1}_{\alpha\alpha_1} H_{\alpha\alpha_2}\rho_{\alpha_2\alpha_1} H_{\alpha_1\alpha'} - S^{-1}_{\alpha_1\alpha'} H_{\alpha\alpha_1}\rho_{\alpha_1\alpha_2} H_{\alpha_2\alpha'}) . \tag{2.21}$$

Thus, $P_{\alpha\alpha'}$ and $P'_{\alpha\alpha'}$, are, respectively, first and second order in H, while $P''_{\alpha\alpha'}$ depends upon the steady-state density matrix ρ. This procedure could be continued, thus generating an expansion in powers of H. However, we shall stop at this point to examine the various terms of the exact Eq. (2.19) in order to determine which are the important ones.

First we note that the density matrix elements in the evaluation of the currents are diagonal in phonon quantum numbers (see Sec. III). Thus the contribution of the phonon scattering V to these elements of $P_{\alpha\alpha'}$ vanishes, as seen from Eqs. (2.18) and (2.5), because V is nondiagonal in phonon quantum numbers. Thus only the electric field part of H "drives" the density matrix elements of interest. The two configurations of interest are the longitudinal one, in which $\vec{E}$ is in the direction of the z axis and for which the diagonal elements are needed, and the transverse case, with $\vec{E}$ along the x axis and for which the needed matrix elements are diagonal in phonon and electron wave numbers, but differ by unity in Landau level n. One finds (see the Appendix)

longitudinal:

$$P_{\alpha\alpha} = [\rho^0, eEz]_{\alpha\alpha} = i\hbar^2 eE\beta m^{*-1}\rho^0_{\alpha\alpha} k_z ; \tag{2.22}$$

transverse:

$$P_{\alpha\bar{\alpha}} = [\rho^0, eEx]_{\alpha\bar{\alpha}} = leE(1 - e^{-s})\rho^0_{\alpha\alpha}[(n+1)/2]^{1/2} . \tag{2.23}$$

Here and below we use $\bar{\alpha}$ to denote the set of quantum numbers identical to the set α except that $\bar{n} = n+1$. The length l is defined in Eq. (A2).

Next we examine $P'_{\alpha\alpha'}$, defined in Eq. (2.20). Using

$$\lim_{\eta \to 0+} S^{-1}_{\alpha\alpha'} = \zeta^*(E_{\alpha\alpha'}) = P(1/E_{\alpha\alpha'}) + i\pi\delta(E_{\alpha\alpha'}) , \tag{2.24}$$

one finds

$$P'_{\alpha\alpha} = 0 , \tag{2.25}$$

$$P'_{\alpha\bar{\alpha}} = \rho^0_{\alpha\alpha} \sum_{\alpha_1} \{[1 - \exp(\beta E_{\alpha\alpha_1})] P(1/E_{\alpha\alpha_1}) - e^{-s}[1 - \exp(\beta E_{\bar{\alpha}\alpha_1})] P(1/E_{\bar{\alpha}\alpha_1})\} H_{\alpha\alpha_1} H_{\alpha_1\bar{\alpha}} . \tag{2.26}$$

To further reduce $P'_{\alpha\bar{\alpha}}$, we drop all terms of second order in $\vec{E}$ since we are interested only in the Ohmic regime in this paper. The terms bilinear in $\vec{E}$ and V vanish because the field term is diagonal in phonon quantum numbers, whereas V is nondiagonal. This leaves just V^2 terms. Most authors

simply discard all terms containing principal-value functions, as in Eq. (2.26), arguing that such terms play no significant role in transport problems. However, in the present case $P'_{\alpha\bar{\alpha}}$ vanishes without that assumption, for the large class of scattering interactions having the property

$$\sum_{k_{1y}}\sum \rho_L(n_{qi})g(\alpha,\alpha_1,\alpha')V_{\alpha\alpha_1}V_{\alpha_1\alpha'}=0 \quad \text{unless } \alpha=\alpha'. \tag{2.27}$$

Here, the second summation is over both phonon quantum number sets $\{n_q\}$ and $\{n_{1q}\}$. Also, $g(\alpha,\alpha_1,\alpha')$ is an arbitrary function, such as that in square brackets in Eq. (2.26), except that it should not be linear in k_{1y} simultaneously with $\alpha'=\alpha$; in that case, the summation is nonzero. A related property, used later, is

$$\sum_{k_{1y}}\sum \rho_L(n_{qi})g(\alpha,\alpha_1,\alpha')V_{\alpha\alpha_1}V_{\bar{\alpha}_1\alpha}=0. \tag{2.28}$$

Again, the arbitrary function $g(\alpha,\alpha_1,\alpha')$ is not linear in k_{1y}. Since the scattering mechanisms considered here satisfy Eq. (2.27), we have the result that $P'_{\alpha\alpha}$ and $P'_{\alpha\bar{\alpha}}$ both vanish, for either the longitudinal or transverse configurations.

Finally, we examine $P''_{\alpha\alpha'}$, defined in Eq. (2.21). Some of its terms are proportional to $\rho_{\alpha\alpha'}$ and can at once be brought to the left side of Eq. (2.19). This step is the principal difference between the present theory and the previous ones which have the divergence difficulties discussed earlier. Those theories in effect replace the $\rho_{\alpha_1\alpha_2}$ in $P''_{\alpha\alpha'}$ by the electric field part of $P_{\alpha_1\alpha_2}/S_{\alpha_1\alpha_2}$, so that $P''_{\alpha\alpha'}$ reduces simply to EV^2 types of terms—the so-called interference terms.[7,9] These are thus Born-approximation theories, going strictly to second order in the scattering potential. The present theory, which retains ρ itself in all terms which seem important, thus goes beyond the Born approximation. Since, as we shall see shortly, the diagonal term $P''_{\alpha\alpha}$ has the familiar gain-loss form and is thus analogous to the Pauli master equation in the time domain, we see that the present technique is evidently equivalent to Van Hove's "V^2t technique"[24] which forms the basis for the derivation of the master equation. (There, the time-dependent density matrix is expanded to all powers of V and time t, and only those terms proportional to some power of V^2t are retained.) Thus we argue that our procedure is logically the one to be used for evaluating the transverse magnetoresistance and other properties requiring off-diagonal density matrix elements, since it is equivalent to that already used in the longitudinal case, where the diagonal elements are needed.

Let us first examine the diagonal elements $P''_{\alpha\alpha}$ for the *longitudinal* case. From Eq. (2.21) we have

$$P''_{\alpha\alpha}=\sum_{\alpha_1}|H_{\alpha\alpha_1}|^2(S^{-1}_{\alpha\alpha_1}+S^{-1}_{\alpha_1\alpha})(\rho_{\alpha\alpha}-\rho_{\alpha_1\alpha_1}) + \text{remaining terms}. \tag{2.29}$$

The separating out of the terms displayed in Eq. (2.29) is permissible since their number is not negligible relative to the number of remaining terms, because of the severe restrictions imposed by the selection rules for the scattering and field terms. This is a manifestation of the so-called Van Hove singularity condition.[24] The displayed term is the familiar gain-loss scattering expression when the Ohmic and $\eta\to 0+$ limits are taken.

To determine the importance of the "remaining terms," one may replace the $\rho_{\alpha_1\alpha_2}$ in them by $P_{\alpha_1\alpha_2}/S_{\alpha_1\alpha_2}$. Then, merely noting that the longitudinal field term eEz has no off-diagonal elements, one sees that all Ohmic terms vanish as $\eta\to 0+$. We conclude that the Ohmic "remaining terms" are of secondary importance even when ρ is retained in them, and shall drop them.

Thus, with use of Eqs. (2.19), (2.22), and (2.24), the needed density matrix elements in the longitudinal case are determined from

$$-2\pi\sum_{\alpha_1}|V_{\alpha\alpha_1}|^2\delta(E_{\alpha\alpha_1})(\rho_{\alpha\alpha}-\rho_{\alpha_1\alpha_1})=\frac{\hbar^2eE\beta k_z\rho^0_{\alpha\alpha}}{m^*} \tag{2.30}$$

in the Ohmic and $\eta\to 0+$ limits. Equation (2.30) is identical to that obtained from the Boltzmann equation. Thus the omitted "remaining terms" constitute small corrections to the Boltzmann equation, and would be the source of, e.g., level-broadening effects.

In calculating the heat and electric currents, the phonon quantum numbers may be summed on first, leaving only electron quantum numbers. Thus it is convenient at this stage to introduce the approximation in which the steady-state density matrix ρ is split into a product of lattice and electron parts. Assuming that the phonon distribution is unaffected by the electric field and the electron-phonon scattering, we write

$$\rho=\rho_L f \tag{2.31}$$

where ρ_L is the equilibrium lattice density matrix of Eq. (2.11), and f is the steady-state electron-density matrix. Note that this decoupling cannot be introduced at the beginning, e.g., in Eq. (2.15), for then the scattering V would vanish when the summation on phonon numbers is carried out. This decoupling also eliminates the effects of phonon drag. We do not mean to imply that phonon drag and the disturbance of the phonon distribution are not important in the present context; in fact, Arora and Miller[1] and many others[12] have shown that they can be important. Instead, our objective here is to display the appropriate transport expressions

for the simplest cases, and to show (Sec. IV) that these expressions are indeed broadly correct in physical consequences and order of magnitude. Refinements such as the above, along with anisotropy of energy surfaces, nonparabolicity of conduction band, etc., can be incorporated when needed.

Using the decoupling in Eq. (2.30), and summing on phonon numbers $\{n_q\}$, we have

$$\sum_{n_1k_1}(w_{nk,n_1k_1}f_{n_1k_1}-w_{n_1k_1,nk}f_{nk})=\hbar eE\beta m^{*-1}k_z f^0_{nk}\ , \tag{2.32}$$

where

$$f_{nk}=\langle nk|\,f\,|nk\rangle\ , \tag{2.33}$$

$$w_{nk,n_1k_1}=\frac{2\pi}{\hbar}\sum_{n_q,n_{1q}}\rho_L(n_{1q})|\,V_{\alpha\alpha_1}|^2\,\delta(E_{\alpha\alpha_1})$$

$$=e^{-\beta(\epsilon_{nk}-\epsilon_{n_1k_1})}w_{n_1k_1,nk}\ , \tag{2.34}$$

and f^0_{nk} is the equilibrium electron-density matrix element given by Eq. (2.12). Under the common assumption that $f_{nk}\propto k_z$, Eq. (2.32) is solved for f_{nk} to give

$$f_{nk}=-\hbar eE\beta m^{*-1}k_z f^0_{nk}\tau'_{nk}\ , \tag{2.35}$$

$$1/\tau'_{nk}=\sum_{n_1k_1}(w_{n_1k_1,nk}-w_{nk,n_1k_1}k_{1z}/k_z) \tag{2.36}$$

Often, as with the scattering interactions considered in this paper, the second term on the right in Eq. (2.36)—the gain term—vanishes because w_{nk,n_1k_1} is an even function of k_{1z}.

Next we turn to the *transverse* case and the quantity $P''_{\alpha\bar{\alpha}}$. From Eq. (2.21),

$$P''_{\alpha\bar{\alpha}}=\rho_{\alpha\bar{\alpha}}\sum_{\alpha_1}(S^{-1}_{\alpha\alpha_1}|\,H_{\bar{\alpha}\alpha_1}|^2+S^{-1}_{\alpha_1\bar{\alpha}}|\,H_{\alpha\alpha_1}|^2)$$

$$+\text{remaining terms.} \tag{2.37}$$

The displayed term is proportional to $\rho_{\alpha\bar{\alpha}}$ and is carried to the left side of Eq. (2.19). Of the "remaining terms," some contain the diagonal density matrix elements in the two forms

$$\rho_{\alpha\alpha}\sum_{\alpha_1}S^{-1}_{\alpha\alpha_1}H_{\alpha\alpha_1}H_{\alpha_1\bar{\alpha}}\quad\text{and}\quad\sum_{\alpha_1}S^{-1}_{\alpha\alpha_1}\rho_{\alpha_1\alpha_1}H_{\alpha\alpha_1}H_{\alpha_1\bar{\alpha}}\ .$$

The Ohmic contribution to the first of these vanishes under the condition (2.27). The second term (as well as the first) is also negligible, since the diagonal density matrix elements themselves are very small in the transverse configuration. There are a number of ways of seeing this. They are not "driven" by the electric field as are the off-diagonal elements $\rho_{\alpha\bar{\alpha}}$; the latter are sufficient to describe both the drift and the Hall currents. Further, the vanishing of both $\rho_{\alpha\alpha}$ and $P'_{\alpha\alpha}$ in the transverse configuration suggest this. Carrying this a step further, one may write out $P''_{\alpha\alpha}$ for the *transverse* case, obtaining the form of Eq. (2.29). When Eq. (2.27) is invoked, all the transverse "remaining terms" depending upon the off-diagonal elements of the field term eEx vanish, leaving just the same terms as in the longitudinal case, which as we have already seen, collectively vanish. Thus only the gain-loss terms remain. Thus Eq. (2.19) becomes in the Ohmic and $\eta\to 0+$ limits

$$0=\sum_{n_1k_1}(w_{nk,n_1k_1}f_{n_1k_1}-w_{n_1k_1,nk}f_{nk})\ , \tag{2.38}$$

which is just the detailed balance condition, resulting in

$$f_{nk}\exp(\beta\epsilon_{nk})=f_{n_1k_1}\exp(\beta\epsilon_{n_1k_1})\ . \tag{2.39}$$

Thus, $f_{nk}\exp(\beta\epsilon_{nk})$ is independent of electron quantum numbers, so that

$$f_{nk}=Ce^{-\beta\epsilon_{nk}}\ . \tag{2.40}$$

Now the equilibrium electron density matrix $\rho_e(H_e)$ has already been properly normalized, requiring that the nonequilibrium part f have the property

$$\sum_{nk}f_{nk}=0\ , \tag{2.41}$$

which is true only if $C=0$. Thus $\rho_{\alpha\alpha}=0$ in the transverse case, under the assumptions stated above.

Going through the same exercises for the "remaining terms" of Eqs. (2.37) which contain off-diagonal elements $\rho_{\alpha_1\alpha_2}$, i.e., replacing the $\rho_{\alpha_1\alpha_2}$ by $P_{\alpha_1\alpha_2}/S_{\alpha_1\alpha_2}$ to estimate the size of the term, one sees that all such terms vanish under the conditions (2.27) and (2.28). Thus Eq. (2.19), with use of Eq. (2.23), becomes in the Ohmic and $\eta\to 0+$ limits

$$E_{\alpha\bar{\alpha}}\rho_{\alpha\bar{\alpha}}=leE(1-e^{-s})^{1/2}[(n+1)/2]^{1/2}\rho^0_{\alpha\alpha}$$

$$+\rho_{\alpha\bar{\alpha}}\sum_{\alpha_1}[\zeta^*(E_{\alpha\alpha_1})|\,V_{\bar{\alpha}\alpha_1}|^2+\zeta^*(E_{\alpha_1\alpha})|\,V_{\alpha\alpha_1}|^2]. \tag{2.42}$$

This is solved for $\rho_{\alpha\bar{\alpha}}$. First carrying out the decoupling procedure, we have

$$(\hbar\Gamma_{nk}-\hbar\omega_c)\langle nk|\,f\,|n+1,k\rangle$$

$$=2^{-1/2}leE(1-e^{-s})(n+1)^{1/2}f^0_{nk}\ , \tag{2.43}$$

where

$$\hbar\Gamma_{nk}=-\sum_{n_1k_1}\sum_{n_qn_{1q}}[\zeta^*(E_{\alpha\alpha_1})|\,V_{\bar{\alpha}\alpha_1}|^2+\zeta^*(E_{\alpha_1\bar{\alpha}})|\,V_{\alpha\alpha_1}|^2]\rho_L(n_q)\ . \tag{2.44}$$

Equations (2.35) and (2.43) are the main results of this section. They have the common form

$$\langle nk|f|n'k\rangle = \frac{C_{nk,n'k}}{\epsilon_{nk}-\epsilon_{n'k}+\hbar\nu_{nn'}(k)-i\hbar/\tau_{nn'}(k)}, \qquad n'=n,n+1 \tag{2.45}$$

for any scattering mechanisms satisfying Eqs. (2.27) and (2.28), and for which $|V_{\alpha\alpha_1}|^2\zeta^*(E_{\alpha\alpha_1})$ is an even function of k_{1z}. Here

$$C_{nk,n'k} = \sum_{\{n_q\}} P_{\alpha\alpha'} \qquad \text{for} \quad \alpha' = n', k, \{n_q\}, \tag{2.46}$$

$$\hbar\nu_{nn'}(k) = -\sum_{\{n_q\}} \rho_L(n_q) \sum_{\alpha_1} [\,|V_{\alpha'\alpha_1}|^2 P(E^{-1}_{\alpha\alpha_1}) + |V_{\alpha\alpha_1}|^2 P(E^{-1}_{\alpha_1\alpha'})\,], \tag{2.47}$$

$$\hbar/\tau_{nn'}(k) = \pi\sum_{\{n_q\}} \rho_L(n_q) \sum_{\alpha_1} [\,|V_{\alpha'\alpha_1}|^2 \delta(E_{\alpha\alpha_1}) + |V_{\alpha\alpha_1}|^2 \delta(E_{\alpha_1\alpha'})\,]. \tag{2.48}$$

Equation (2.45) is the solution, for the desired matrix elements, to what may be called the quantum Boltzmann equation (2.19), where $P_{\alpha\alpha'}$ is the drift term and $P''_{\alpha\alpha'}$ is the scattering term. We note that Γ_{nk} of Eqs. (2.43) and (2.44), from which $\nu_{nn'}(k)$ and $\tau_{nn'}(k)$ are defined, is equivalent to $\Gamma_\alpha(0)$ in the cyclotron-resonance-linewidth theory of Kawabata.[25] There, $1/\tau_{nn'}(k)$ contributes to the width and $\nu_{nn'}(k)$ to the shift of the cyclotron resonance line.

With the results of the Appendix, we note that for the two types of scattering considered explicitly in Sec. IV (as well as some others, e.g., short-range impurity scattering[25]), Eqs. (2.47) and (2.48) further reduce to

$$\nu_{nn'}(k) = \tfrac{1}{2}(\nu_{nk} - \nu_{n'k}), \tag{2.49}$$

$$1/\tau_{nn'}(k) = \tfrac{1}{2}(\tau^{-1}_{nk} + \tau^{-1}_{n'k}), \tag{2.50}$$

where

$$\nu_{nk} = -\frac{2}{\hbar}\sum_{\{n_q\}} \rho_L(n_q) \sum_{\alpha_1} |V_{\alpha\alpha_1}|^2 P(E^{-1}_{\alpha\alpha_1}), \tag{2.51}$$

$$\tau^{-1}_{nk} = \frac{2\pi}{\hbar}\sum_{\{n_q\}} \rho_L(n_q) \sum_{\alpha_1} |V_{\alpha\alpha_1}|^2 \delta(E_{\alpha\alpha_1}). \tag{2.52}$$

Equation (2.50) shows that the off-diagonal relaxation rate is the average of the relaxation rates out of the two states separately, a property which has been noted previously for electron scattering on random impurities[25,26] or acoustic phonons,[25,27] and for spin-spin relaxation.[26] Equation (2.49) shows that the off-diagonal energy shift is one-half the difference of two terms. The calculations of Sec. IV show that scattering on acoustic phonons makes no contribution to the energy shift,[25] but that scattering with emission of an optic phonon does.

The presence of the $\nu_{nn'}(k)$ and $1/\tau_{nn'}(k)$ terms in the denominator of Eq. (2.45) provide a Breit-Wigner[28] type of relation for the density matrix, with the "energy shift" $\nu_{nn'}$ and "collision broadening" $1/\tau_{nn'}$ occurring naturally. Many authors[29-31] have achieved a form similar to Eq. (2.45) by artificially adding a relaxation term $(\rho_0-\rho)/\tau$ to the right side of the Liouville Eq. (2.8) while not attempting to extract the information from the commutator term. The present paper shows how to do this more accurately.

III. MAGNETOTRANSPORT COEFFICIENTS

To illustrate the use of the theory developed in Sec. II, we shall evaluate several magnetotransport coefficients. Since the conventions used for defining these coefficients vary so widely in the literature,[5,32,33] and since a consistent sign convention is necessary in the evaluation of the magneto-Seebeck tensor components, we shall briefly develop some relations among the coefficients.

The linear response (electric current density $\vec{J}$ and total energy flux density $\vec{W}$) to electric and thermal driving forces may be written, in the notation of Pavlov and Firsov[33,34]

$$\vec{J} = \underline{\alpha}\cdot\vec{E}^* - \underline{\beta}\cdot\nabla T, \tag{3.1}$$

$$\vec{F} \equiv \vec{W} + \zeta e^{-1}\vec{J} = \underline{\gamma}\cdot\vec{E}^* - \underline{\chi}\cdot\nabla T, \tag{3.2}$$

where $\vec{E}^*$ is a sum of the applied field $\vec{E}$ and the field generated by the electrons because of an inhomogeneous temperature and electron distribution:

$$\vec{E}^* = \vec{E} + e^{-1}\nabla\zeta(\vec{B}, n_e, T). \tag{3.3}$$

The absolute thermoelectric power, or magneto-Seebeck coefficient $\underline{\alpha}$ is defined by

$$\vec{E}^* = \underline{\alpha}\cdot\nabla T, \tag{3.4}$$

with the subsidiary condition $\vec{J}=0$. The absolute Peltier coefficient $\underline{\pi}$ ($-\underline{\pi}$ in Jan's notation[32]) is defined by

$$\vec{F} = \underline{\pi}\cdot\vec{J}, \tag{3.5}$$

with the subsidiary condition $\nabla T = 0$. The Seeback and Peltier coefficients are connected by the Kelvin relation[5]

$$\pi_{ij}(\vec{B}) = T\alpha_{ji}(-\vec{B}). \tag{3.6}$$

Equations (3.1) and (3.2) together with (3.4) and (3.5) show that

$$\underline{\beta} = \underline{\sigma}\circ\underline{\alpha} \tag{3.7}$$

$$\underline{\gamma} = \underline{\pi} \cdot \underline{\sigma} \,. \tag{3.8}$$

The Kelvin relation (3.6), together with the Onsager relation

$$L_{ij}(\vec{B}) = L_{ji}(-\vec{B}) \,, \tag{3.9}$$

where $L(\vec{B})$ represents any of the above tensors, then shows that $\underline{\beta}$ and $\underline{\gamma}$ are related by

$$\underline{\gamma} = T\underline{\rho} \circ \underline{\beta} \cdot \underline{\sigma} \,, \tag{3.10}$$

where $\underline{\rho}$ is the resistivity tensor, inverse to the conductivity tensor $\underline{\sigma}$.

For isotropic systems with the magnetic field in the z direction, which is what we are considering, the tensors are additionally antisymmetric and have the common form[5]

$$\underline{L} = \begin{pmatrix} L_1 & -L_2 & 0 \\ L_2 & L_1 & 0 \\ 0 & 0 & L_3 \end{pmatrix} . \tag{3.11}$$

Equation (3.10) then reduces to

$$\underline{\gamma}(\vec{B}) = T\underline{\beta}(\vec{B}) \,. \tag{3.12}$$

We shall evaluate the magnetoresistivity tensor $\underline{\rho}(\vec{B})$ and the magneto-Seebeck tensor $\underline{\alpha}(\vec{B})$, since they are commonly measured quantities. One finds their components to be, noting the form (3.11) as well as $\underline{\rho} = \underline{\sigma}^{-1}$ and Eq. (3.7),

$$\rho_1 = \sigma_1/S \tag{3.13}$$

$$\rho_2 = -\sigma_2/S \,, \tag{3.14}$$

$$\rho_3 = 1/\sigma_3 \,, \tag{3.15}$$

$$\alpha_1 = (\sigma_1\beta_1 + \sigma_2\beta_2)/S \,, \tag{3.16}$$

$$\alpha_2 = (\sigma_1\beta_2 - \sigma_2\beta_1)/S \,, \tag{3.17}$$

$$\alpha_3 = \beta_3/\sigma_3 \,, \tag{3.18}$$

where

$$S = \sigma_1^2 + \sigma_2^2 \,. \tag{3.19}$$

The reason for introducing the relation (3.12) is so that we may evaluate $\underline{\gamma}$ rather than $\underline{\beta}$ in computing the Seebeck tensor $\underline{\alpha}$, since $\underline{\gamma}$ occurs for $\nabla T = 0$, and the problems associated with introducing a temperature gradient into the Hamiltonian formulation are thereby avoided.

The electric and energy current densities are determined by use of the density matrix from the statistical-mechanical prescription

$$\vec{J} = \mathrm{Tr}(\rho \vec{J}_{op}) \,, \tag{3.20}$$

$$\vec{F} = \mathrm{Tr}(\rho \vec{F}_{op}) \,, \tag{3.21}$$

where the associated operators are given by[35]

$$\vec{J}_{op} = -e\vec{v} \,, \tag{3.22}$$

$$F_{op} = \tfrac{1}{2}[(H_e - \zeta)\vec{v} + \vec{v}(H_e - \zeta)] \,. \tag{3.23}$$

The matrix elements of $\vec{v}$ are given in the Appendix.

From Eqs. (3.1), (3.2), (3.12), (3.16)–(3.23), and (2.45)–(2.48), one finds

$$\sigma_1 = \frac{e^2}{m^*}(1 - e^{-s}) \sum_{n,k} (n+1) f^0_{nk} g_{nk} \,, \tag{3.24}$$

$$\sigma_2 = \frac{e^2}{m^*}(1 - e^{-s}) \sum_{n,k} (n+1) f^0_{nk} g'_{nk} \,, \tag{3.25}$$

$$\sigma_3 = \frac{e^2\hbar^2\beta}{m^{*2}} \sum_{n,k} k_z^2 \tau_{nn}(k) f^0_{nk} \,, \tag{3.26}$$

$$\beta_1 = \frac{\zeta\sigma_1}{eT} - \frac{e}{m^*T}(1 - e^{-s}) \times \sum_{n,k} (n+1) f^0_{nk}(\epsilon_{nk} + \tfrac{1}{2}\hbar\omega_c) g_{nk} \,, \tag{3.27}$$

$$\beta_2 = \frac{\zeta\sigma_2}{eT} - \frac{e}{m^*T}(1 - e^{-s}) \times \sum_{n,k} (n+1) f^0_{nk}(\epsilon_{nk} + \tfrac{1}{2}\hbar\omega_c) g'_{nk} \,, \tag{3.28}$$

$$\beta_3 = \frac{\zeta\sigma_3}{eT} - \frac{e\hbar^2\beta}{m^{*2}T} \sum_{n,k} k_z^2 \tau_{nn}(k) f^0_{nk} \epsilon_{nk} \,, \tag{3.29}$$

where

$$g_{nk} = \tau^{-1}_{n,n+1}(k)/D_{n,n+1}(k) \,, \tag{3.30}$$

$$g'_{nk} = [\omega_c - \nu_{n,n+1}(k)]/D_{n,n+1}(k) \,, \tag{3.31}$$

$$D_{n,n+1}(k) = [\omega_c - \nu_{n,n+1}(k)]^2 + \tau^{-2}_{n,n+1}(k) \,. \tag{3.32}$$

The resistivity and Seebeck tensor components are determined from the above equations with the use of Eqs. (3.13)–(3.19). The results of some numerical computations are shown in the next section.

The expressions for the longitudinal components σ_3 and β_3, as given in Eqs. (3.26) and (3.29), are the same as those obtained earlier[34,36] by use of the Boltzmann equation generalized to include magnetic fields and Landau quantization. This is because the theory of the previous section reduces to the Boltzmann equation in the longitudinal case, as discussed there. The transverse conductivity expression (3.24) is equivalent to the zero-frequency limit of the cyclotron resonance expressions of Kawabata[25] and Ito *et al.*,[27] who used different means of derivation. Our results are convergent even when the relaxation rates (proportional to $|V|^2$) diverge, which occurs for electrons making transitions to the Landau subband edges.

It is of interest to note that the expressions (3.24)–(3.29) correctly reduce in the $\vec{B} \to 0$ limit to the zero-field Boltzmann-equation results. That is, σ_2 and β_2 vanish, and $\sigma_1 \to \sigma_3 \to \sigma(0)$, $\beta_1 \to \beta_3 \to \beta(0)$, where

$$\sigma(0) = ZF_0(\gamma, 0) \,, \tag{3.33}$$

$$\beta(0) = \frac{\zeta(0)\sigma(0)}{eT} - \frac{k_B}{e} ZF_1(\gamma, 0) \,, \tag{3.34}$$

where

$$Z=\frac{4n_e e^2\hbar^4(2\pi\beta)^{1/2}\rho_d u_l^2}{3E_{op}^2\hbar\omega_0\langle n_0\rangle m^{*5/2}}\,, \tag{3.35}$$

$$F_n(\gamma,0)=\int_0^\infty \frac{dx\,e^{-x}x^{n+3/2}}{Cx^{1/2}+(x+\gamma)^{1/2}+e^{\gamma}(x-\gamma)^{1/2}}\,, \tag{3.36}$$

$$C=2/[\langle n_0\rangle\gamma(E_{op}/E_{ac})^2]\,, \tag{3.37}$$

$$\gamma=\beta\hbar\omega_0\,. \tag{3.38}$$

Here, E_{op} and E_{ac} are deformation potential energies corresponding to the optic and acoustic phonons, and $\langle n_0\rangle$ is the thermal number of optic phonons of frequency ω_0. Thus, when acoustic phonon scattering dominates, $\sigma(0)$ becomes Z/C, which, when Eqs. (3.35)–(3.38) are used, is seen to be the usual zero-field expression for this type of scattering. Also for this case, the normalized Hall coefficient

$$r_H\equiv -n_e eR_H=-n_e e\rho_{yx}/B\,, \tag{3.39}$$

which is close to unity at high fields, takes the usual value[37] $\frac{3}{8}\pi$ as $B\to 0$. The Seebeck coefficient in this case becomes

$$\alpha(0)=\frac{\beta(0)}{\sigma(0)}=-\frac{k_B}{e}\left(2-\frac{\zeta(0)}{k_B T}\right), \tag{3.40}$$

which is the standard result,[37] independent of the scattering. (It should be noted, however, that in the presence of the inelastic optic phonon scattering, the zero-field expressions for r_H and α do not take these simple forms, and are scattering dependent.) The Ettingshausen-Nernst coefficient for pure acoustic phonon scattering becomes, as $B\to 0$,

$$\frac{\alpha_{yx}}{B}\to\frac{3\pi k_B}{16n_e e^2}\frac{Z}{C}\,. \tag{3.41}$$

The earlier theories for transverse magnetoresistance, having the divergence difficulties, do not extrapolate to the correct $B=0$ results, being essentially high-field theories.

Finally, we note that if $\nu_{n,n+1}(k)$ in Eqs. (3.24)–(3.26) is ignored, and the relaxation times $\tau_{n,n+1}(k)$ and $\tau_{n,n}(k)$ are taken as constant or replaced by suitably averaged quantities, the familiar expressions[3,5]

$$\sigma_{xx}=\sigma_1=\frac{n_e e^2}{m^*}\frac{\tau}{1+(\omega_c\tau)^2}\,, \tag{3.42}$$

$$\sigma_{yx}=\sigma_2=\frac{n_e e^2}{m^*}\frac{\omega_c\tau^2}{1+(\omega_c\tau)^2}\,, \tag{3.43}$$

$$\sigma_{zz}=\sigma_3=\frac{n_e e^2\tau}{m^*}\,, \tag{3.44}$$

are obtained from Eqs. (3.24)–(3.26). The familiar phenomenological resistivity components then result from Eqs. (3.13)–(3.15). Applying the same approximation to the $\underline{\beta}$ tensor, and then evaluating the Seebeck tensor $\underline{\alpha}$ from Eqs. (3.16)–(3.18), one finds the not-so-familiar expressions

$$\alpha_1=\frac{\zeta}{eT}-\frac{k_B}{e}\left(\frac{1}{2}+s\coth\frac{s}{2}\right), \tag{3.45}$$

$$\alpha_2=0\,, \tag{3.46}$$

$$\alpha_3=\frac{\zeta}{eT}-\frac{k_B}{e}\left(\frac{3}{2}+\frac{s}{2}\coth\frac{s}{2}\right). \tag{3.47}$$

The Ettingshausen-Nernst term α_2 thus vanishes in this approximation, while the transverse and longitudinal Seebeck coefficients, α_1 and α_2, are independent of scattering mechanism. The differences between these phenomenological expressions and those containing the details of the scattering are discussed in the next section.

IV. NUMERICAL CALCULATIONS

We illustrate the theory developed in Sec. II by calculating the magnetotransport coefficients of Sec. III for purely elastic scattering on acoustic phonons, and for combined scattering on acoustic and optic phonons, the latter giving rise to the magnetophonon effect.

First, a few remarks about the relaxation-time and energy shift terms are in order. The relaxation rate for the combined scattering is the sum of the separate rates, and may be written

$$\frac{1}{\tau_n(k)}=\sum_i A_i\sum_{m=-\infty}^{n}[(z^2+\gamma_i+sm)^{-1/2}+e^{\gamma_i}(z^2-\gamma_i+sm)^{-1/2}]\,, \tag{4.1}$$

where the sum on i refers to the acoustic and optic phonon scatterings, and

$$A_{op}=\frac{E_{op}^2\hbar\omega_0\langle n_0\rangle s}{2\rho_d u_l^2\pi\hbar^4}\left(\frac{m^{*3}}{2\beta}\right)^{1/2}, \tag{4.2}$$

$$A_{ac}=\tfrac{1}{2}A_{op}C\,, \tag{4.3}$$

$$\gamma_{op}=\gamma=\beta\hbar\omega_0\,, \tag{4.4}$$

$$\gamma_{ac}=0\,, \tag{4.5}$$

$$z^2=\beta\hbar^2k_z^2/2m^*\,. \tag{4.6}$$

The quantity C in Eq. (4.3) is defined in Eq. (3.37). The expression (4.5) is a result of equipartition for the acoustic phonons:

$$\langle n_q\rangle+1=e^{\beta\hbar\omega_q}\langle n_q\rangle\approx\langle n_q\rangle\approx(\beta\hbar\omega_q)^{-1}\,. \tag{4.7}$$

The quantity $[\tau_{n,n+1}(k)]^{-1}$ appearing in the off-diagonal density-matrix expression is the arithmetic mean of the two rates $1/\tau_n(k)$ and $1/\tau_{n+1}(k)$.

The energy-shift term may be written

$$\nu_n(k)=\sum_i A_i\sum_{m=-\infty}^{n}[(-z^2-\gamma_i-sm)^{-1/2}+e^{\gamma_i}(-z^2+\gamma_i-sm)^{-1/2}]\,. \tag{4.8}$$

Now $\nu_{n,n+1}(k)$ is one-half the *difference* of two shifts, according to Eq. (2.49). Noting that $x^{-1/2}$

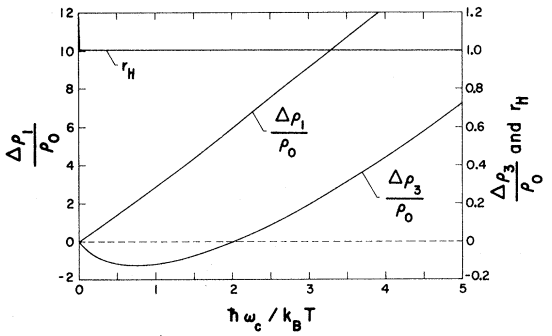

FIG. 1. Transverse (subscript 1) and longitudinal (subscript 3) magnetoresistance and Hall coefficient as a function of magnetic field for elastic scattering on acoustic phonons. Deformation potential $E_{ac}=10$ eV. Temperature $=\frac{1}{3}\Theta=94$ K.

$\equiv 0$ whenever $x<0$, one finds

$$\nu_{n,n+1}(k) = -\tfrac{1}{2}A_{op}e^{\gamma}[\gamma - s(n+1) - z^2]^{-1/2} . \qquad (4.9)$$

Thus, the acoustic phonon scattering makes no contribution to the line shift, as noted earlier by Kawabata.[25] Further, only the emission term of the optic phonon scattering contributes to the line shift.

Figure 1 shows the longitudinal and transverse magnetoresistance, and the normalized Hall coefficient r_H of Eq. (3.39), for purely deformation-potential acoustic phonon scattering. We have used parameter values similar to those of n-InSb in all the figures: $\Theta \equiv \hbar\omega_0/k_B = 281$ K, $m^* = 0.016 m_e$, $\rho_d = 5780$ kg/m^3, $u_l = 3700$ m/sec, and $E_{ac} = 8$–10 eV. The deviation of r_H from unity is indeed very small in the figure. However, r_H rises to $3\pi/8$ at $B=0$, the rise beginning only at about $s=\beta\hbar\omega_c = 0.01$. The transverse magnetoresistance is of particular importance here, and has a range of values quite representative of many substances.[2,38] Of course, the curves are not meant to describe quantitatively any particular material; they do show, however, that the theory as developed, with its natural cutoff, gives correct order-of-magnitude results without any extra assumptions. This is not to suggest that, e.g., level broadening considerations may not be important, because of course in some circumstances they are, e.g., in analyzing the amplitudes of the various magneto-oscillatory phenomena. The point we wish to make here is that level broadening *per se* is not necessary to make the transverse magnetoresistance finite or of the correct magnitude. The "natural" theory is able to do this. Within it, level broadening can be incorporated as in the divergent theories.

The interesting region of negative longitudinal magnetoresistance seen in Fig. 1 perhaps deserves some comment. As we have stated earlier, the underlying formula, Eq. (3.26), is the usual one, and can be found in many papers, perhaps the earliest being that of Argyres.[39] However, Dubinskaya[40] was apparently the first to recognize that it gives a region of negative magnetoresistance for deformation-potential scattering on acoustic phonons. Our previous work[36] confirmed this, and has shown a region of negative longitudinal magnetoresistance for nonpolar optic phonon scattering as well. Dubinskaya gave the physical reason, which, in somewhat more detail, is as follows: For $\hbar\omega_c \ll k_B T$, i.e., small fields, or equivalently, high temperatures, there are many (elastic) scattering processes which can end near $k_z = 0$, near the bottom of a Landau subband. These processes are very effective in limiting the mobility because they correspond to very small relaxation times. As the field increases from its small values, fewer of these processes contribute, because Landau levels are passing up out of the populated energy region, and the mobility increases (resistance decreases). When $\hbar\omega_c \gtrsim k_B T$, the last of these processes ceases to be significant. For higher fields, the scattering details become unimportant; the available electrons now are progressively crowded nearer $k_z = 0$ in the bottom Landau level, and contribute less to the mobility, meaning that the resistance now increases. This physical argument seems to be quite general, and suggests that impurity scattering should show a similar behavior.

For the reader who may be thinking that the negative longitudinal magnetoresistance at low "classical" fields is inconsistent with the old classical theory (see, e.g., Ref. 5) which gives zero longitudinal magnetoresistance, we point out that there, not only are the magnetic-field effects not quantized, but also the relaxation time is assumed to be independent of magnetic field. If the latter assumption is made in the present theory, it too will give no longitudinal magnetoresistance.

Figure 2 shows the analogous results (purely

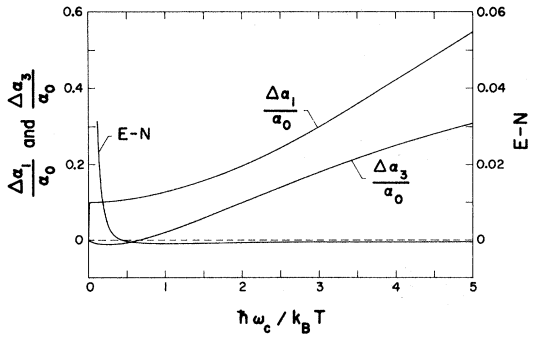

FIG. 2. Magneto-Seebeck components as a function of magnetic field, for the same conditions as in Fig. 1, and $n_e = 5\times10^{14}$ cm^{-1}. "E-N" is the Ettingshausen-Nernst coefficient α_{yx}/B divided by $\hbar/m^*T = 77$ μV/K T $= 7.7 \times 10^{-5}$ m^2/K sec.

acoustic phonon scattering) for the magnetothermal components. We show the longitudinal and transverse Seebeck coefficients as well as the dimensionless quantity $e\alpha_2/sk_B = eT\alpha_2/\hbar\omega_c$, which is proportional to the Ettingshausen-Nernst coefficient α_{yx}/B. Again, these coefficients are of the correct order of magnitude.[38,41,42] It is useful to note how well these curves approximate the phenomenological expressions (3.45)–(3.47) in the high-field region. The longitudinal Seebeck coefficient is seen to have about half the slope of the transverse coefficient, in agreement with Eqs. (3.45) and (3.47), and to lie approximately the prescribed distance below it. The Ettingshausen-Nernst coefficient is indeed very small at high fields, in agreement with Eq. (3.46), but rises to the positive value given by Eq. (3.41), appropriate to acoustic phonon scattering. An experimental result shows this qualitative behavior,[42] but the positive value is there ascribed to impurity scattering. The transverse Seebeck coefficient $\Delta\alpha_1/\alpha(0)$ of Fig. 2 seems to approach the zero-field axis at a finite value, but in fact turns toward the origin at $s \approx 0.01$, about where the Hall coefficient makes its turn. The experimental result of Muzhdaba *et al.*[41] shows such an elbow.

In Fig. 3, we show the magnetoresistivity with combined acoustic and optic phonon scattering at a temperature equivalent to 77 K in InSb. The transverse magnetoresistance shows resonance maxima which are finite in amplitude, but larger than observed experimentally in any material. The latter shows the need for inclusion of level-broadening techniques for an analysis of resonance amplitudes. The longitudinal magnetoresistance shown in Fig. 3 shows the resonance minima, pseudoresonance minima, and off-resonance maxima which have been discussed in detail earlier.[2,36]

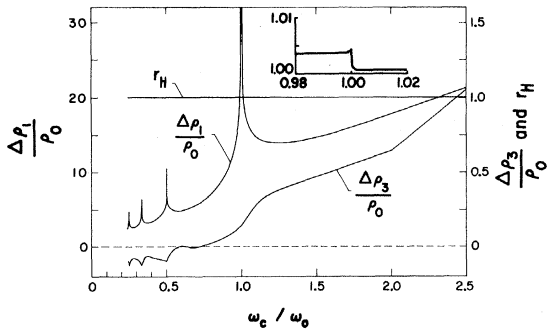

FIG. 3. Magnetoresistance as a function of magnetic field for combined scattering on acoustic ($E_{ac} = 8$ eV) and optic ($E_{op} = 24$ eV) phonons, with $T = \Theta/3.66 = 77$ K, showing magnetophonon structure in the transverse and longitudinal magnetoresistance. Magnetophonon structure is also present in the Hall coefficient but is very small; as shown in the inset, it has a steplike character.

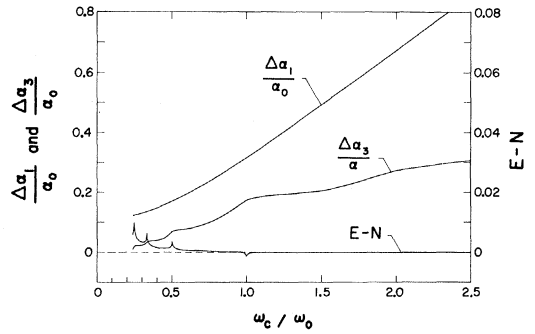

FIG. 4. Magneto-Seebeck components as a function of magnetic field, for the same conditions as in Fig. 3, and $n_e = 6.2 \times 10^{13}$ cm^{-3}. No magnetophonon structure is discernible in the transverse component; broad off-resonance maxima and very small slope discontinuities at the resonance and pseudoresonance fields are seen in the longitudinal component; sharp features occur at the resonance fields in the Ettingshausen-Nernst coefficient.

Finally, the Hall coefficient shows almost no structure. The structure which exists is rather steplike, as shown on a greatly expanded scale in the inset. In view of the smallness of these steps and the expectation that level broadening would smear them out considerably, it is somewhat surprising that magnetophonon oscillations have been observed experimentally[43,44] in the Hall voltage.

Figure 4 shows the magnetophonon structure in the magnetothermal coefficients, for the same parameter values as in Fig. 3. The longitudinal Seebeck coefficient α_3 is similar to curves published earlier,[34] and qualitatively similar to several observations,[2,34] showing principally the broad off-resonance maxima, and scarcely discernible pseudoresonance and resonance maxima (actually, slope discontinuities). No structure is seen in the transverse Seebeck coefficient α_1, but there is very pronounced structure in α_2. One should note the remarkable inverted amplitude at $\omega_c = \omega_0$ in the calculated Ettingshausen-Nernst coefficient in Fig. 4. Calculations for other temperatures and ratios of elastic to inelastic scattering show that this inversion relative to the lower-field amplitudes persists. To date, there has been only one report of observed magnetophonon oscillations in the Ettingshausen-Nernst coefficient.[42] There, the second and third peaks, corresponding to $N = 2$ and 3 in the resonance condition $N\omega_c = \omega_0$, were observed in n-InSb, and were maxima, in agreement with Fig. 4. The experiment was not carried to fields high enough to observe the $N = 1$ peak, and so whether it is a maximum or minimum is still not known.

To sum up, the theory presented here gives a straightforward way of calculating magnetotransport coefficients without encountering the tradi-

tional divergence difficulties. The results for the transverse magnetoconductivity are identical to some earlier results of cyclotron-resonance theory extrapolated to zero frequency. The theory in the limit of small magnetic fields agrees with conventional zero-field results. The expressions for the magnetotransport coefficients have the "natural cutoff" form. The theory has permitted the first detailed calculation of magnetophonon effects in the transverse magnetoresistance, the Hall coefficient, and the Ettingshausen-Nernst coefficient.

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APPENDIX

The eigenfunctions of the electron Hamiltonian (2.2) are

$$\psi_{nk} = \exp[i(k_y y + k_z z)]\phi_n((x - x_k)/l)/(L_y L_z)^{1/2}, \quad \text{(A1)}$$

where the single index k denotes the pair (k_y, k_z), and L_y, L_z are sample dimensions. The $\phi_n((x-x_k)/l)$ are harmonic-oscillator functions centered at $x_k = -l^2 k_y$, where

$$\phi_n(y) = (2^n n!\, l\pi^{1/2})^{-1/2} H_n(y)\, e^{-y^2/2}, \quad \text{(A2)}$$

$$l^2 = \hbar/m^* \omega_c, \quad \text{(A3)}$$

and $H_n(y)$ is a Hermite polynomial.

The matrix elements of the velocity operator

$$\vec{v} = i\hbar^{-1}[H_T, \vec{r}] = i\hbar^{-1}[H_e, \vec{r}] \quad \text{(A4)}$$

between states $\psi_{n'k'}$ and ψ_{nk} are

$$\langle n'k' | v_x | nk\rangle = (il\omega_c/2^{1/2}) \times [(n+1)^{1/2}\delta_{n',n+1} - n^{1/2}\delta_{n',n-1}]\delta_{k'k}, \quad \text{(A5)}$$

$$\langle n'k' | v_y | nk\rangle = (l\omega_c/2^{1/2}) \times [(n+1)^{1/2}\delta_{n',n+1} + n^{1/2}\delta_{n',n-1}]\delta_{k'k}, \quad \text{(A6)}$$

$$\langle n'k' | v_z | nk\rangle = (\hbar k_z/m^*)\delta_{n'n}\delta_{k'k}. \quad \text{(A7)}$$

The quantities $P_{\alpha\alpha'}$ defined in Eq. (2.18) may be written

$$P_{\alpha\alpha'} = (\rho^0_{\alpha\alpha} - \rho^0_{\alpha'\alpha'})V_{\alpha\alpha'} + [\rho^0, e\vec{E}\cdot\vec{r}]_{\alpha\alpha'}. \quad \text{(A8)}$$

The electric field term $[\rho, e\vec{E}\cdot\vec{r}]$ is diagonal in phonon quantum numbers. The following matrix elements are used in the evaluation of the field term for the longitudinal and transverse configurations:

$$\langle n'k' | [f^0(H_e), z] | nk\rangle = (i\hbar^2\beta/m^*) f^0_{nk} k_z \delta_{n'n}\delta_{k'k} \quad \text{(A9)}$$

$$\langle n'k' | [f^0(H_e), x] | nk\rangle = \frac{\hbar^2 f^0_{nk}}{2^{1/2} m^* l} \frac{1 - \exp[\beta\hbar\omega_c(n'-n)]}{\hbar\omega_c(n'-n)} \times [(n+1)^{1/2}\delta_{n',n+1} - n^{1/2}\delta_{n',n-1}]\delta_{k'k}. \quad \text{(A10)}$$

The matrix elements of the position operator x are also used. These are

$$\langle n'k' | x | nk\rangle = -l^2 k_y \delta_{n'n}\delta_{k'k} + l\,2^{-1/2} \times [(n+1)^{1/2}\delta_{n',n+1} + n^{1/2}\delta_{n',n-1}]\delta_{k'k}. \quad \text{(A11)}$$

The matrix elements of the electron portion $e^{i\vec{q}\cdot\vec{r}}$ of the scattering term are

$$\langle n'k' | e^{i\vec{q}\cdot\vec{r}} | nk\rangle = \delta_{q,k'-k} J_{n'n}(q_x, k'_y, k_y), \quad \text{(A12)}$$

where

$$J_{n'n}(q_x, k'_y, k_y) = \int_{-\infty}^{\infty} dx\, e^{iq_x x} \phi_{n'}\left(\frac{x + l^2 k'_y}{l}\right)\phi_n\left(\frac{x + l^2 k_y}{l}\right). \quad \text{(A13)}$$

The following property of $J_{n'n}$ is used in this paper:

$$\int_{-\infty}^{\infty} dq_x \int_{-\infty}^{\infty} dq_y\, J_{n'n}(q_x, k'_y, k_y) J_{nn'}(-q_x, k_y, k'_y) = 2\pi/l^2. \quad \text{(A14)}$$

The left-hand side of Eq. (A14) occurs with deformation potential scattering when equipartition, linear dispersion ($\omega_q = qu_l$), and collision elasticity are assumed for acoustic phonons, and no dispersion ($\omega_q = \omega_0$) is assumed for optic phonons. It also results for other interactions with certain approximations; e.g., scattering on screened ionized impurities can be cast into the form of Eq. (2.6) with a coupling coefficient proportional to $(q^2 + r_s^{-2})^{-1}$ where r_s is a screening length. If here $q_x^2 + q_y^2$ is approximated by a parameter such as l^{-2}, then the combination on the left side of Eq. (A14) results. Any scattering mechanism with this characteristic also satisfies Eqs. (2.27) and (2.28).

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