Effect of electron-phonon drag on the magnetoconductivity tensor of n-germanium

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A density-matrix formalism is developed to calculate the magnetoconductivity tensor in semiconductors, taking into account the mutual electron-phonon drag. An application of the formalism is made to the four-ellipsoidal model of n-germanium under the conditions where acoustic-phonon scattering is the predominant mechanism of scattering and the high-temperature limit of the phonon distribution is valid. The magnitude of the relaxation effects of secondary interactions for electrons and for phonons is found by making comparison with the existing experimental data. It is suggested that scattering of electrons by transitions to bound impurity states plays an important role in the case of transverse magnetoresistance.

I. INTRODUCTION

The study of the effects of magnetic fields on the transport properties of semiconductors provides useful information about the role various scattering mechanisms play in the presence of external fields. While the theory for longitudinal magnetoresistance[1] agrees well with experiments for n-type germanium,[2] assuming that acoustic-phonon scattering is predominant, similar agreement for transverse magnetoconduction proves to be elusive.[3,4] In spite of a large amount of theoretical work,[5,6] only a few attempts[1,3,7] have been made to provide a comparison with the existing experimental data. This has been partly because of the belief of some authors[8] that the effect of inhomogeneities may be larger than those of fundamental scattering mechanisms in the transverse case. Recent experiments by Baranskii and Babich[9,7] lead to the conclusion that there is very little correlation between inhomogeneities and transverse magnetoresistance. It is suggested in the present paper that the difficulty with previous calculations is in the neglect of the nonequilibrium, anisotropic phonon distribution due to electron drag.

The mutual entrainment effect of the coupled electron-phonon system was discussed by Sommerfeld and Bethe.[10] Sondheimer[11] emphasized the importance of formulating the problem in such a way as to preserve symmetry between the electron and phonon systems as far as mutual interaction is concerned. Hubner and Shockley[12] experimentally observed the creation of an electric current due to phonon drag. Recently the disturbance of the optical-phonon distribution in InSb has been demonstrated by Kranzer and Gornick.[13] Gurevich *et al.*[14] have shown theoretically that the temperature and magnetic field dependence of magnetoresistance changes if mutual entrainment of the electron and phonon systems is taken into account.

In the case of transverse magnetoresistance, the anisotropic phonon distribution arises due to drag by electrons which tend to have a drift velocity resulting from the crossed electric and magnetic fields. If there were no interactions other than conduction electron-phonon scattering, the phonons would be isotropic not in the crystal frame but in a frame moving with the electron drift velocity, provided that the drift velocity was small compared to the sound velocity. The electrons would then tend to relax isotropically in the drift-velocity frame. Hence the current would not be affected by the scattering. Thus to explain transverse magnetoresistance effects, one must consider secondary scattering mechanisms. Additional phonon interactions could change the frame in which the phonons are isotropic. Additional electron interactions could cause the electrons to relax to some intermediate velocity frame.

Another departure from other treatments is to split the electric field $\vec{\mathcal{E}}$ into two parts: one part is treated exactly in finding the unperturbed basis functions, while the other part is used as a perturbation. Ordinarily when phonon anisotropy is not considered, the transverse electric field has either been included completely in the unperturbed Hamiltonian[3,15,16] or has been used completely as a perturbation.[17] These two approaches give quite different results. The perturbation approach gives for the transverse current Eq. (4.5) of this paper, with the parameter γ appearing there set equal to zero. On the other hand, inclusion of $\vec{\mathcal{E}}$ in the unperturbed Hamiltonian with later expansion for small $\vec{\mathcal{E}}$ leads to Eq. (4.5) with $\gamma = 1$, together with other terms involving derivatives of the distribution function such as in Eq. (3.31). These results are different both for high and low magnetic fields. In particular, the latter result, in which $\vec{\mathcal{E}}$ is in the unperturbed Hamiltonian, diverges at low magnetic fields. This divergence may result from expansion in powers of $1/\omega\tau$,[15,16] but there is still a divergence when $\omega\tau$ is not assumed large.[3] How-

ever, when the electric field is treated as a perturbation, there is no such divergence and the expression goes into that for the usual low-field transverse current found from the Boltzmann transport equation. The difficulties when the basis quantum functions include the electric field arise for the same reason that difficulties occur when classical motion in crossed electric and magnetic fields is used as the unperturbed motion in the Boltzmann transport equation. In both cases one can solve the transport equations exactly and, regardless of other small interactions, the distribution function is found to contain $\exp(-e\vec{\mathcal{E}}\cdot\vec{r}/kT)$. It is then not consistant to expand to first order for small $\vec{\mathcal{E}}$. Thus if one wishes to investigate linear effects in $\vec{\mathcal{E}}$, this field must ordinarily be treated as small from the start.

However, in the calculations in Sec. III below the anisotropic part of the phonon distribution is shown to give effects similar to those occurring when $\vec{\mathcal{E}}$ is included in the unperturbed Hamiltonian. Then if the electric field were treated completely as a perturbation, this anisotropic phonon distribution would give a nonuniform spatial distribution for the electrons. To avoid this difficulty, one must include a sufficient part of the electric field in the unperturbed Hamiltonian to cancel this anisotropic effect. If there is no longitudinal current due to this part of the electric field and the anisotropic phonon distribution, there is no tendency for the electrons to become nonuniformly distributed. Thus that part of the longitudinal current (not including that due to the remaining perturbing electric field) will be set equal to zero as the criterion used in deciding on the division of $\vec{\mathcal{E}}$ into the two parts.

In Sec. II the basic perturbation treatment of the density matrix is presented. This is a modification of the formalism of Argyres[15] and that of Adams and Holstein.[16] This density matrix is evaluated in Sec. III using the wave functions for the energy ellipsoids of n-Ge. The results are given and discussed in Sec. IV. Also in that section suggested mechanisms for the secondary scattering are discussed.

II. DENSITY MATRIX FOR COUPLED ELECTRON-PHONON SYSTEM

The basic physical quantity of interest here is the expectation value of the current operator $\vec{j}$:

$$\langle\vec{j}\rangle = \mathrm{Tr}(\rho_T\vec{j}) \ , \tag{2.1}$$

where ρ_T is the density matrix for the coupled electron-phonon system. For small coupling and for small deviations of the density matrix from equilibrium we may assume that ρ_T is of the form

$$\rho_T = (\rho_0^e + \rho^e)(\rho_0^{ph} + \rho^{ph}) \ , \tag{2.2}$$

where ρ_0^e and ρ_0^{ph} are the unperturbed electron and phonon parts of the density matrix. The quantities ρ^e and ρ^{ph} are the corresponding corrections due to the switching on of a perturbation. The corrections ρ^e and ρ^{ph} can be obtained by solving Liouville's equation:

$$\frac{\partial\rho_T}{\partial t} = -\frac{i[\mathcal{H}_T, \rho_T]}{\hbar} \ , \tag{2.3}$$

where $\mathcal{H}_T$ is the total electron and phonon Hamiltonian:

$$\mathcal{H}_T = \mathcal{H}_0 + \mathcal{H}' \tag{2.4}$$

with

$$\mathcal{H}_0 = \mathcal{H}_e + \mathcal{H}_L + \gamma F_\perp, \quad 0 \le \gamma \le 1 \ , \tag{2.5}$$

$$\mathcal{H}' = V + I + F' \ , \tag{2.6}$$

$$F' = (1-\gamma)F_\perp + F_\parallel \ . \tag{2.7}$$

Here $F_\perp$ is the interaction involving the part of the electric field which is transverse to the magnetic field and $F_\parallel$ is that involving the electric field parallel to the magnetic field. The quantity $\mathcal{H}_L$ is the lattice part of the Hamiltonian. The potential V is the electron-phonon interaction taken to be[18] (for unit volume)

$$V = iE_1\sum_q\left(\frac{\hbar}{2\rho_d\omega_q}\right)^{1/2} q(a_q + a_{-q}^\dagger)\, e^{i\vec{q}\cdot\vec{r}} \ , \tag{2.8}$$

where $a_q^\dagger$ is the acoustic-phonon creation operator for wave vector $\vec{q}$, a_q is an annihilation operator, ρ_d is the crystal mass density, and ω_q is the frequency of a phonon. No distinction between longitudinal and transverse phonons will be considered here, and they will be treated as longitudinal.[1] The potential energy I in the Hamiltonian consists of any other interaction responsible for electron or phonon relaxation. As discussed in the Introduction, if I were not included, the current would be the same as that which would occur with no scattering at high magnetic fields.

The parameter γ will be chosen such that when the perturbation F' of Eq. (2.5) is set equal to zero, the density matrix corresponds to an equilibrium uniform electron distribution. When the electron distribution is being calculated the phonon distribution will be assumed independent of γ. Eventually the phonon distribution must be chosen consistent with the choice of γ. As will be seen in the formalism below, the anisotropic phonon distribution due to electron drag acts effectively as an additional transverse electric field tending to give the electrons a drift velocity equal to the velocity of the frame in which phonon distribution appears isotropic. The competition between this effect and the interactions I and γF can, with proper choice of γ, give zero current parallel to the electric field. If this component of current is zero,

there is no tendency for electrons to collect in low-potential-energy regions, and there is a uniform equilibrium electron distribution. The part of the electric field interaction, F', which leads to a non-equilibrium distribution is then treated as a perturbation.

Likewise in finding the anisotropic phonon distribution, it will be assumed that the electron current is known and is independent of the phonon distribution. Competition between the electron drag and that due to any interaction I will lead to the phonon anisotropy. As mentioned above, consistency between this anisotropy and the choice of γ is then imposed as a condition on the overall density matrix.

It is now desired to find ρ^e of Eq. (2.2), the change in the electron distribution due to perturbations. For this treatment a density matrix[19] is taken of the form

$$\rho_T^e = \rho_0 + \rho e^{st} \quad , \tag{2.9}$$

where ρ_0 and ρe^{st} are, respectively, ρ_0^e and ρ^e times $\mathrm{Tr}(\rho_0^{ph} + \rho^{ph})$. It is assumed here that ρ^{ph} is given; i.e., in addition to the perturbations discussed above, there is a perturbation that acts on the phonons only to hold ρ^{ph} constant. This perturbation becomes zero at $t = 0$. The quantity ρe^{st} is the correction to ρ_0 when a perturbation is switched on slowly over the time interval $t = -\infty$ to $t = 0$:

$$\mathcal{H}'(t) = e^{st}\mathcal{H}' \quad , \tag{2.10}$$

where s is a small positive parameter. The problem is then to calculate $\rho_T^e(t)$ at $t = 0$ in the limit $s \to 0$. Substitution of Eqs. (2.9) and (2.10) into (2.3) yields

$$(E_{\nu'\nu} - ihs)\,\rho_{\nu'\nu} = \rho_{0\nu'\nu}(V+I)_{\nu'\nu} + [\rho, V+I]_{\nu'\nu}e^{st} + C_{\nu'\nu} \tag{2.11}$$

with

$$C_{\nu'\nu} = [\rho_0, F']_{\nu'\nu} \quad , \tag{2.12}$$

$$\rho_{0\nu'\nu} = \rho_{0\nu'} - \rho_{0\nu} \quad , \tag{2.13}$$

$$E_{\nu'\nu} = E_{\nu'} - E_{\nu} \quad . \tag{2.14}$$

Here $\rho_{0\nu}$ is the diagonal part of the initial density matrix and E_ν is the energy eigenvalue corresponding to a state characterized by a set of quantum numbers ν. In Eq. (2.11) $[\rho, F]$ has been neglected, as only those parts of ρ which are linear in electric field are retained. Solving the above Eq. (2.11) for $\rho_{\nu'\nu}$ and substituting back on the right-hand side, one obtains the result

$$(E_{\nu'\nu} - ihs)\,\rho_{\nu'\nu} = C_{\nu'\nu} + \rho_{0\nu'\nu}(V+I)_{\nu'\nu} + \sum_{\nu''} \frac{C_{\nu'\nu''} + \rho_{0\nu'\nu''}(V+I)_{\nu'\nu''} + [\rho, V+I]_{\nu'\nu''}e^{st}}{E_{\nu'\nu''} - ihs}(V+I)_{\nu''\nu}e^{st}$$

$$-\sum_{\nu''}(V+I)_{\nu'\nu''}\frac{C_{\nu''\nu} + \rho_{0\nu''\nu}(V+I)_{\nu''\nu} + [\rho, V+I]_{\nu''\nu}e^{st}}{E_{\nu''\nu} - ihs}e^{st} \quad . \tag{2.15}$$

Now one takes the limit $s \to 0$ and uses the relationship:

$$\lim_{s\to 0}(x - is)^{-1} = P(1/x) + i\pi\delta(x) \quad . \tag{2.16}$$

The part $P(1/x)$ is the principal value which does not contribute to reversible current effects[16] and hence will be dropped. Furthermore, one can take an ensemble average in which case terms linear in V or I will go to zero. Also terms involving I multiplied by ρ will be dropped since acoustic-phonon scattering will be considered predominant. The result is

$$E_{\nu'\nu}\rho_{\nu'\nu} = C_{\nu'\nu} + i\pi\sum_{\nu''}[\rho_{0\nu'\nu''}\,\delta(E_{\nu'\nu''}) + \rho_{0\nu\nu''}\,\delta(E_{\nu\nu''})](V_{\nu'\nu''}V_{\nu''\nu} + I_{\nu'\nu''}I_{\nu''\nu})$$

$$+ i\pi\sum_{\nu''\nu'''}(\rho_{\nu'\nu''}V_{\nu''\nu'''}V_{\nu'''\nu} - V_{\nu'\nu''}\rho_{\nu''\nu'''}V_{\nu'''\nu})\,\delta(E_{\nu'\nu''})$$

$$- i\pi\sum_{\nu''\nu'''}(V_{\nu'\nu''}\rho_{\nu''\nu'''}V_{\nu'''\nu} - V_{\nu'\nu''}V_{\nu''\nu'''}\rho_{\nu'''\nu})\,\delta(E_{\nu\nu''}) \quad . \tag{2.17}$$

To proceed further, one must introduce specific electron eigenfunctions of the unperturbed Hamiltonian $\mathcal{H}_e + \gamma F_\perp$ of Eq. (2.5).

III. WAVE FUNCTIONS AND ELECTRON DENSITY MATRIX

For n-Ge the four energy minima are ellipsoids of revolution with the axes of revolution along the four directions equivalent to the [111] direction. The total current will be the sum of the currents for these ellipsoids. For the calculations the coordinate axes will be oriented such that the applied magnetic field $\vec{B}$ is along the positive z axis and $\vec{\mathcal{E}}_\perp$, the part of the electric field perpendicular to $\vec{B}$, is along the positive x axis. Then the unperturbed

one-electron Hamiltonian for any one energy ellipsoid is

$$\mathcal{H} = \mathcal{H}_e + \gamma F_\perp = \sum_{i,j} \frac{\alpha_{ij}}{2m}\left(p_i + \frac{e}{c}A_i\right)\left(p_j + \frac{e}{c}A_j\right) + e\gamma\mathcal{E}_\perp x \quad , \tag{3.1}$$

where m and e are electronic mass and magnitude of electronic charge, respectively. In this Hamiltonian, the interaction between the magnetic field and the electronic magnetic moment can be ignored for the field strengths considered in the present work. The vector potential $\vec{A}$ giving the uniform applied field $\vec{B}$ will be chosen in the Landau gauge $\vec{A} = (0, Bx, 0)$. It will be assumed that $\vec{B}$, parallel to z axis, is at an angle θ relative to the longitudinal ellipsoidal axis and that $\vec{\mathcal{E}}$, parallel to the x axis, is at angle ϕ relative to the plane containing $\vec{B}$ and the ellipsoidal axis. If θ and ϕ were zero, the reciprocal mass tensor α_{ij}/m would be diagonal with elements which will be designated by α_1/m, α_1/m, α_3/m. In general, however,

$$\alpha = \begin{pmatrix} a_{11}\cos^2\phi + \alpha_1\sin^2\phi & (a_{11}-\alpha_1)\sin\phi\cos\phi & a_{13}\cos\phi \\ (a_{11}-\alpha_1)\sin\phi\cos\phi & a_{11}\sin^2\phi + \alpha_1\cos^2\phi & a_{13}\sin\phi \\ a_{13}\cos\phi & a_{13}\sin\phi & \alpha_{33} \end{pmatrix} \quad , \tag{3.2}$$

with

$$a_{11} = \alpha_1\cos^2\theta + \alpha_3\sin^2\theta \quad , \tag{3.3}$$

$$a_{13} = (\alpha_1 - \alpha_3)\sin\theta\cos\theta \quad , \tag{3.4}$$

$$\alpha_{33} = \alpha_1\sin^2\theta + \alpha_3\cos^2\theta \quad . \tag{3.5}$$

The eigenfunctions of the Hamiltonian (3.1), normalized in a unit volume, are[3]

$$\Psi_{nk} = \exp[i(k_y y + k_z z) - i(\gamma_{13}k_z + \gamma_{12}k_y)x - i\gamma_{12}x^2/2\lambda^2]\,\phi_n(\beta(x - x_k)) \quad , \tag{3.6}$$

where in terms of the Hermite polynomials H_n,

$$\phi_n(\beta(x-x_k)) = (\beta/\pi^{1/2}2^n n!)^{1/2}\exp[-\beta^2(x-x_k)^2/2] \times H_n(\beta(x-x_k)) \quad , \tag{3.7}$$

with

$$\beta = \frac{(\alpha_1 a_{11}/\alpha_{11}^2)^{1/4}}{\lambda} \quad , \qquad \lambda = (\hbar c/eB)^{1/2} \quad , \qquad \gamma_{12} = \alpha_{12}/\alpha_{11} \quad , \qquad \gamma_{13} = \alpha_{13}/\alpha_{11} \tag{3.8}$$

and

$$x_k = -\lambda^2\left(k_y + \frac{\alpha_{23}k_z}{a_{11}}\right) - \frac{\alpha_{11}m}{\alpha_1 a_{11}e\gamma\mathcal{E}_\perp}\left(\frac{c\gamma\mathcal{E}_\perp}{B}\right)^2 \quad . \tag{3.9}$$

The energy eigenvalues are

$$E_{nk} = \epsilon_{nk} + \frac{\frac{1}{2}\alpha_{11}m(c\gamma\mathcal{E}/B)^2}{\alpha_1 a_{11}} + e\gamma\mathcal{E}_\perp x_k \quad . \tag{3.10}$$

Here

$$\epsilon_{nk} = (n + \tfrac{1}{2})\hbar\omega^* + \hbar^2 k_z^2/2m^* \quad , \qquad n = 0, 1, 2, \ldots \quad , \tag{3.11}$$

with

$$\omega^* = (eB/mc)(\alpha_1 a_{11})^{1/2} \quad , \qquad 1/m^* = \alpha_1\alpha_3/a_{11}m \quad . \tag{3.12}$$

In these expressions, the symbol k stands for k_y, k_z. The Greek subscripts in Eq. (2.17) stand for n, k_y, k_z.

Also, the one-phonon Hamiltonian has eigenvalues $(N_q + \frac{1}{2})\omega_q$. These energies must be included in the E_ν of Eq. (2.14). It will be assumed that $\vec{q}$ is small enough so that $\omega_q = uq$ with u an average sound velocity. Since the characteristic lengths associated with the magnetic fields and with the temperatures considered here are of the order of 10^{-6} cm, the $\vec{q}$'s of importance are of the order 10^6 cm^{-1}.

The matrix elements of the one-electron current operators,

$$j_i = -ev_i = -ie[\mathcal{H}, r_i]/\hbar \quad , \tag{3.13}$$

with the above representation as a basis are given by

$$\langle n'k'|j_x|nk\rangle = \alpha_{11}j_1(n'k', nk) \quad , \tag{3.14}$$

$$\langle n'k'|j_y|nk\rangle = \alpha_{12}j_1(n'k', nk) + j_2(n'k', nk) \quad , \tag{3.15}$$

$$\langle n'k'|j_z|nk\rangle = \alpha_{13}j_1(n'k', nk) + (\alpha_{23}/a_{11})j_2(n'k', nk) + j_3(n'k', nk) \quad , \tag{3.16}$$

where

$$j_1(n'k', nk) = (i\hbar e\beta/m)\{[(n+1)/2]^{1/2}\delta_{n',n+1} - (n/2)^{1/2}\delta_{n',n-1}\}\delta_{k'k} \quad , \tag{3.17}$$

$$j_2(n'k', nk) = -[\hbar e\beta(\alpha_1 a_{11})^{1/2}/m]\{[(n+1)/2]^{1/2}\delta_{n',n+1} + (n/2)^{1/2}\delta_{n',n-1}\}\delta_{k'k} + (ec\gamma\mathcal{E}_\perp/B)\delta_{n'n}\delta_{k'k} \tag{3.18}$$

$$j_3(n'k', nk) = -(e\hbar k_z/m^*)\delta_{n'n}\delta_{k'k} \quad . \tag{3.19}$$

Since the average current involves $\mathrm{Tr}(\vec{j}\rho_T^e)$, it is clear from Eqs. (3.14)–(3.19) that only the diagonal parts of ρ_T^e and the parts of the form $\rho_{nk,(n\pm1)k}$ need be found. Also, these are the large parts of

ρ_T^e because the driving terms of Eq. (2.17), the first two terms on the right-hand side, are large only for $n'=n$, $n\pm1$ and $k'=k$. For instance, one term, the $C_{\nu'\nu}$ of Eq. (2.12), is

$$C_{n'k',nk}=\rho_{0n'k',nk}[(1-\gamma)e\mathcal{E}_\perp x+e\mathcal{E}_z z]_{n'k',nk}=\frac{e}{\sqrt{2}\beta}\rho_{0n'k',nk}\left[\left((1-\gamma)\mathcal{E}_\perp+\frac{\alpha_{13}\mathcal{E}_z}{\alpha_{11}}\right)[(n+1)^{1/2}\delta_{n',n+1}+n^{1/2}\delta_{n',n-1}]\right.$$
$$\left.-i\frac{\alpha_{23}\sqrt{\alpha_1}\mathcal{E}_z}{\alpha_{11}\sqrt{a_{11}}}[(n+1)^{1/2}\delta_{n',n+1}-n^{1/2}\delta_{n',n-1}]\right]\delta_{k',k}+i\left(\frac{-\hbar^2 e\mathcal{E}_z k_z}{m^*}+\frac{\alpha_{23}\lambda^2\gamma e^2\mathcal{E}_\perp\mathcal{E}_z}{a_{11}}\right)\frac{d\rho_{0nk}}{d\epsilon_{nk}}\delta_{n',n}\delta_{k',k}\ . \quad (3.20)$$

The other driving term will be discussed below.

Let us now consider the terms in Eq. (2.17) involving matrix elements of the electron-phonon interaction V. The matrix elements of the creation or annihilation operator $a_q^\dagger$, a_q of Eq. (2.8) will lead to a factor N_q+1 or N_q in each of these terms for emission or absorption of a phonon, respectively. These will be replaced by the average value

$$\langle N_q\rangle=\{\exp[\hbar(\omega_q+\vec{v}\cdot\vec{q})/k_B T]-1\}^{-1}\ . \quad (3.21)$$

This anisotropic expression differs from the equilibrium expression through the term $\vec{v}\cdot\vec{q}$ where $\vec{v}$ is the velocity, relative to the lattice, of the frame in which the phonons appear to have an approximately isotropic distribution. Thus $\vec{v}\cdot\vec{q}$ is essentially a Doppler frequency shift. If there were only electron-phonon interactions with no interactions I and with $\mathcal{E}_z=0$, γ would be equal to unity and both $\vec{v}$ and electron drift velocity averaged over the ellipsoids would have components $[0, c\mathcal{E}_\perp/B, 0]$. In the high-temperature approximation, which will be used here,

$$\langle N_q\rangle\simeq\langle N_q+1\rangle\simeq k_B T/[\hbar(\omega_q+\vec{v}\cdot\vec{q})]$$
$$\simeq(k_B T/\hbar\omega_q)(1-\vec{v}\cdot\vec{q}/\omega_q) \quad (3.22)$$

for $v\ll u$, the sound speed. From the integrals over the coordinates, the matrix elements $V_{nk,n'k'}$ for a given $\vec{q}$ will also have for phonon absorption or emission a factor $\delta_{k_y',k_y\pm q_y}\delta_{k_z',k_z\pm q_z}$ times a function of the $\vec{q}$ components expressible in terms of associated Laguerre polynomials.[20] Two useful sum rules for isotropic phonon distribution are[16]

$$\sum_{k_y'}V_{nk,mk'}V_{m'k',n'k}=C\delta_{n',n} \quad (3.23)$$

with C independent of n and m;

$$\sum_{m,k_y'}(K_1 q_y+K_2 q_z)V_{nk,mk'}V_{mk',(n+1)k}$$
$$=K_1(\sqrt{2}\beta\lambda^2)^{-1}(n+1)^{1/2}\sum_\lambda|V_{nk,\lambda}|^2 \quad (3.24)$$

for K_1 and K_2 constants and for $q_y=k_y-k_y'$, $q_z=k_z-k_z'$.

If elastic scattering were assumed (that is, $\hbar\omega_q$ and thus also $e\gamma\mathcal{E}_\perp x_k$ and $\vec{v}\cdot\vec{q}$ negligible), Eq. (3.23) could be used to simplify some of the terms in Eq. (2.17). Thus a term such as $V_{nk,mk'}\rho_{mk',m'k'}\times V_{m'k',(n\pm1)k}$ would be zero. Then since parts of ρ not diagonal in k are assumed negligible, terms containing $(V\rho V)_{nk,(n\pm1)k}$ could be dropped. Similar arguments based on the diagonal part of ρ being odd in k_z apply to terms containing $(V\rho V)_{nk,nk}$. Likewise, in those summations involving $\rho_{\nu'\nu''}\times V_{\nu''\nu'''}V_{\nu'''\nu}$, Eq. (3.23) would eliminate all but $\rho_{\nu'\nu}V_{\nu\nu'''}V_{\nu'''\nu}$. However, if inelastic scattering is considered, the scattering is not isotropic and terms dropped are not zero. Nevertheless, these terms will still be small and can still be dropped for temperatures considered here. Then one can solve Eq. (2.17) for $\rho_{\nu'\nu}$:

$$\rho_{\nu'\nu}=\left(C_{\nu'\nu}+i\pi\sum_{\nu''}[\rho_{0\nu'\nu''}\delta(E_{\nu'\nu''})+\rho_{0\nu\nu''}\delta(E_{\nu\nu''})]\right.$$
$$\left.\times\frac{V_{\nu'\nu''}V_{\nu''\nu}+I_{\nu'\nu''}I_{\nu''\nu}}{\epsilon_{\nu'\nu}-i\hbar/\tau_{\nu'\nu}}\right)\ , \quad (3.25)$$

where

$$1/\tau_{\nu'\nu}=\tfrac{1}{2}(1/\tau_{\nu'}+1/\tau_\nu) \quad (3.26)$$

with

$$\frac{1}{\tau_\nu}=\frac{2\pi}{\hbar}\sum_{\nu''}|V_{\nu,\nu''}|^2\delta(\epsilon_{\nu,\nu''})\ . \quad (3.27)$$

For elastic scattering the evaluation of C in Eq. (3.23) using Eq. (2.8) would lead to[1]

$$\frac{1}{\tau_{nk}}=\frac{E_1^2 k_B T(2m^*)^{1/2}}{\pi\hbar^2\rho_d u^2\lambda^2}\sum_{n'}[\epsilon_{nk}-(n'+\tfrac{1}{2})\hbar\omega^*]^{-1/2}\ . \quad (3.28)$$

The summation over n' is over only those values such that $\epsilon_{nk}-(n'+\frac{1}{2})\hbar\omega^*>0$. Because of the neglect of inelasticity, the $1/\tau_{nk}$ of Eq. (3.28) approaches infinity as $k_z\to0$ owing to the term where $n'=n$. This would not lead to an infinity in $\rho_{\nu'\nu}$ since $1/\tau_{nk}$ occurs in the denominator of Eq. (3.25). However, neglect of inelasticity can lead to incorrect numerical results. Therefore in the term of Eq. (3.27) for which $n'=n$, $\pm\hbar\omega_q$ was included in the δ function for phonon absorption and emission, respectively. Since ω_q depends on $\vec{q}$, the sum over the $\vec{q}$'s had to be done numerically by computer. In the other terms for which $n'\neq n$, the effect of

inelastic scattering is small if $\omega^* \gg \omega_q$.

Next we consider the numerator of Eq. (3.25). An expression for $C_{\nu'\nu}$ has already been given in Eq. (3.20). To simplify the rest of the terms in the numerator, one must choose $\rho_{0\nu}$. As discussed previously it is desirable to have $\rho_{0\nu}$ correspond to a uniform distribution of electrons independent of the position in the x direction. Therefore for nondegenerate statistics $\rho_{0\nu}$ will be chosen to be a Boltzmann distribution involving ϵ_{nk} of Eq. (3.11), not the total electron energy E_{nk} of Eq. (3.10):

$$\rho_{0nk} = \exp[(\mu - \epsilon_{nk})/k_B T] , \tag{3.29}$$

with

$$e^{\mu/k_B T} = (2\pi\lambda)^2 N(B)\left[\sum_p \left(\frac{2\pi m_p^* k_B T}{\hbar^2}\right)^{1/2} \times \operatorname{csch}\left(\frac{\hbar\omega_p^*}{2k_B T}\right)\right]^{-1} , \tag{3.30}$$

independent of position. Thus local thermodynamic equilibrium is assumed. Here, $N(B)$ is the density of conduction electrons, which, according to Minner,[21] can be approximated by its zero-field value for the range of parameters used here. The subscript p stands for the energy ellipsoid being considered. Since the δ functions in Eq. (3.25) involve the energy of Eq. (3.10) as well as phonon energy, the quantities $\rho_{0\nu'\nu''} = \rho_{0\nu'} - \rho_{0\nu''}$ will in general not be zero. Thus let us consider one of the terms of Eq. (3.25) containing $\rho_{0\nu'\nu''}$,

$$i\pi \sum_{\nu''} \rho_{0\nu'\nu''} V_{\nu'\nu''} V_{\nu''\nu} \delta(E_{\nu'\nu''}) .$$

For phonon absorption and with $h\omega_q / k_B T \ll 1$ some of the factors under the summation are

$$\left(1 - \frac{\vec{v}\cdot\vec{q}}{\omega_q}\right)\rho_{0\nu'\nu''}\,\delta(E_{\nu'\nu''}) \simeq \left[\hbar(\omega_q - \vec{v}\cdot\vec{q}) + \frac{\gamma c\mathcal{E}_\perp \hbar}{B} \times \left(q_y + \frac{\alpha_{23} q_z}{a_{11}}\right)\right] \frac{d\rho_{0n'k'}}{d\epsilon_{n'k'}}\,\delta(\epsilon_{\nu'\nu''}) . \tag{3.31}$$

The first factor on the left-hand side is an anisotropy coming from the quadratic $V_{\nu'\nu''} V_{\nu''\nu}$ due to the phonon distribution, Eq. (3.22). If in Eq. (3.25) $\rho_{\nu'\nu} = \rho_{nk',(n+1)k}$, Eq. (3.23) indicates that to a good approximation the isotropic parts may be dropped, and the anisotropic parts are approximately proportional to $1/\tau_{nk}$ according to Eq. (3.24). It is seen that the result is also proportional to the difference between the velocity $\vec{v}$ of the isotropic phonon frame and the electron drift velocity due to $\gamma\mathcal{E}_\perp$. Phonon emission gives a similar result. Also, the term involving $\rho_{0\nu\nu''}$ gives a similar result with $-d\rho_{0(n+1)k}/d\epsilon_{(n+1)k}$ replacing the derivative in Eq. (3.31).

The terms involving the interaction I will be assumed to have no anisotropic $\vec{q}$ dependence. Then again for $\rho_{nk,(n+1)k}$, these terms will be proportional to a reciprocal relaxation time, $1/\tau_I^e$, times the drift velocity of the electrons (no $\vec{v}\cdot\vec{q}$ term in this case). As discussed previously γ is chosen so that these driving terms with perturbation $C_{\nu'\nu}$ set equal to zero give zero current in the x direction. This leads to a relationship of the form

$$\frac{v_y - \gamma c\mathcal{E}_\perp/B}{\gamma c\mathcal{E}_\perp B} = R_e , \tag{3.32}$$

with

$$R_e = \frac{\langle 1/\tau_I^e\rangle_{av}}{\langle 1/\tau_{nk}^e\rangle_{av}} . \tag{3.33}$$

The notation $\langle\cdots\rangle_{av}$ around the reciprocal relaxation times indicates an average weighted by the x component of current operator and the other factors in the density matrix of Eq. (3.25).

To find another equation for v_y and γ, one may treat the phonon density matrix. In this case the electron distribution including current flow is assumed to be known and constant as e^{st} goes from zero to unity. Here the electron current density $\vec{j}$ tends to drag the phonons along with a velocity $\vec{v}' = \vec{j}/Ne$ where N is the electron particle density. One obtains an equation like (3.25) but with no $C_{\nu'\nu}$. In this case, terms quadratic in matrix elements of V and presumably I are diagonal in phonon quantum numbers and thus only diagonal density-matrix components are large. If ρ_0 for the phonons is chosen to be that of Eq. (3.21), one may set $\rho_{\nu'\nu} = 0$. Then the driving terms in the equivalent of Eq. (3.25) must be zero. This results in the relationship

$$\frac{v_y' - v_y}{v_y} = R_p = \frac{1/\tau_I^q}{1/\tau_q} . \tag{3.34}$$

Here τ_q is the phonon relaxation time due to conduction-electron–phonon interaction (assumed predominant) and τ_I^q is a phonon relaxation time due to any other interactions I. R_p will be a function of $\vec{q}$, but it is assumed approximately constant over the small range of $\vec{q}$'s of importance here. Equations (3.32) and (3.34) lead to

$$\gamma = \frac{v_y'/(c\mathcal{E}_\perp/B)}{1+R} , \tag{3.35}$$

with

$$1 + R = (1 + R_e)(1 + R_p) . \tag{3.36}$$

This γ varies as B^2 for small magnetic field. Once γ is chosen in this manner, only $C_{\nu'\nu}$ need be retained as a driving term in Eq. (3.25).

IV. RESULTS AND DISCUSSION

By taking the traces of j_1, j_2, j_3 in Eqs. (3.17)–(3.19) using the density matrix of Eq. (3.25), one

finds that for a given energy ellipsoid the current components may be written in terms of the three conductivities,

$$\sigma_1 = \frac{e^2}{m}\sum_{nks}\frac{\rho_{0nk}(1-e^{-a})(n+1)(1/\tau_{nk,(n+1)k})}{\omega^{*2}+(1/\tau_{nk,(n+1)k})^2} \quad , \tag{4.1}$$

$$\sigma_2 = \frac{e^2}{m}\sum_{nks}\frac{\rho_{0nk}(1-e^{-a})(n+1)\omega^*}{\omega^{*2}+(1/\tau_{nk,(n+1)k})^2} \quad , \tag{4.2}$$

$$\sigma_3 = -e^2\sum_{nks}\tau_{nk}\left(\frac{\hbar k_z}{m^*}\right)^2\frac{d\rho_{0nk}}{d\epsilon_{nk}} \quad , \tag{4.3}$$

with

$$a = \hbar\omega^*/k_B T \quad .$$

To first order in the electric field $\vec{\mathcal{E}}$,

$$\langle j_x\rangle = \alpha_{11}\sigma_1(1-\gamma)\mathcal{E}_\perp + [\alpha_{13}\sigma_1 - \alpha_{23}(\alpha_1/a_{11})^{1/2}\sigma_2]\mathcal{E}_z \quad , \tag{4.4}$$

$$\langle j_y\rangle = [\alpha_{12}\sigma_1 + (\alpha_1 a_{11})^{1/2}\sigma_2](1-\gamma)\mathcal{E}_\perp + \gamma Nec\mathcal{E}_\perp/B + [\alpha_{23}\sigma_1 + (\alpha_1/a_{11})^{1/2}\alpha_{13}\sigma_2]\mathcal{E}_z \quad , \tag{4.5}$$

$$\langle j_z\rangle = [\alpha_{13}\sigma_1 + (\alpha_1/a_{11})^{1/2}\alpha_{23}\sigma_2](1-\gamma)\mathcal{E}_\perp + \alpha_{23}\gamma Nec\mathcal{E}_\perp/\alpha_{11}B + (\sigma_3 + a_{13}^2\sigma_1/a_{11})\mathcal{E}_z \quad . \tag{4.6}$$

The total conductivity is found by summing Eqs. (4.4)–(4.6) over the four energy ellipsoids. For a general direction of $\vec{\mathcal{E}}$ one may write $\langle j_i\rangle = \sum_l \sigma_{il}\mathcal{E}_l$. This conductivity tensor σ_{il} and thus the resistivity tensor may be formed by noting that σ_2 changes sign under time reversal while σ_1 and σ_3 do not. The primary effect of the electron-phonon drag is to decrease the transverse magnetoconductivity by a factor, $1-\gamma$, compared to the result one would obtain using an equilibrium phonon distribution. The magnetoconductivity tensor can be inverted to give for the magnetoresistivity tensor components, ρ_{xx} and ρ_{xy}, when $\vec{B}$ is along a direction of symmetry:

$$\rho_{xx} = \sigma_{yy}/(\sigma_{xx}\sigma_{yy} + \sigma_{xy}^2) \quad , \tag{4.7}$$

$$\rho_{xy} = \sigma_{yx}/(\sigma_{xx}\sigma_{yy} + \sigma_{xy}^2) \quad . \tag{4.8}$$

The quantities frequently measured in an experiment are the Hall coefficient, related to ρ_{xy}, and the ratio $\rho_{xx}(B)/\rho(0)$ where $\rho(0)$ is the zero-field resistivity.[1]

Results of the calculations of transverse magnetoresistance for n-Ge are shown in Figs. 1 and 2. For these calculations the constants used were $\alpha_1 = 12.2$, $\alpha_3 = 0.633$, $E_1 = 12.5$ eV, and $N = 3.7\times10^{13}$ cm^{-3}, assuming the effect of the magnetic field on the number of conduction electrons is negligible.[21] In Fig. 1, the ratio $\rho_{xx}^{(B)}/\rho_0$ is shown as a function of magnetic field. The solid curves are from the experiments of Gallagher and Love.[4] The dashed curves are the theoretical results if no asymmetry in the phonon distribution is taken into account, i.e., if $\gamma = 0$. In Fig. 2 are shown the corresponding parameters R of Eq. (3.36) necessary for theoretical results to fit the experimental values.

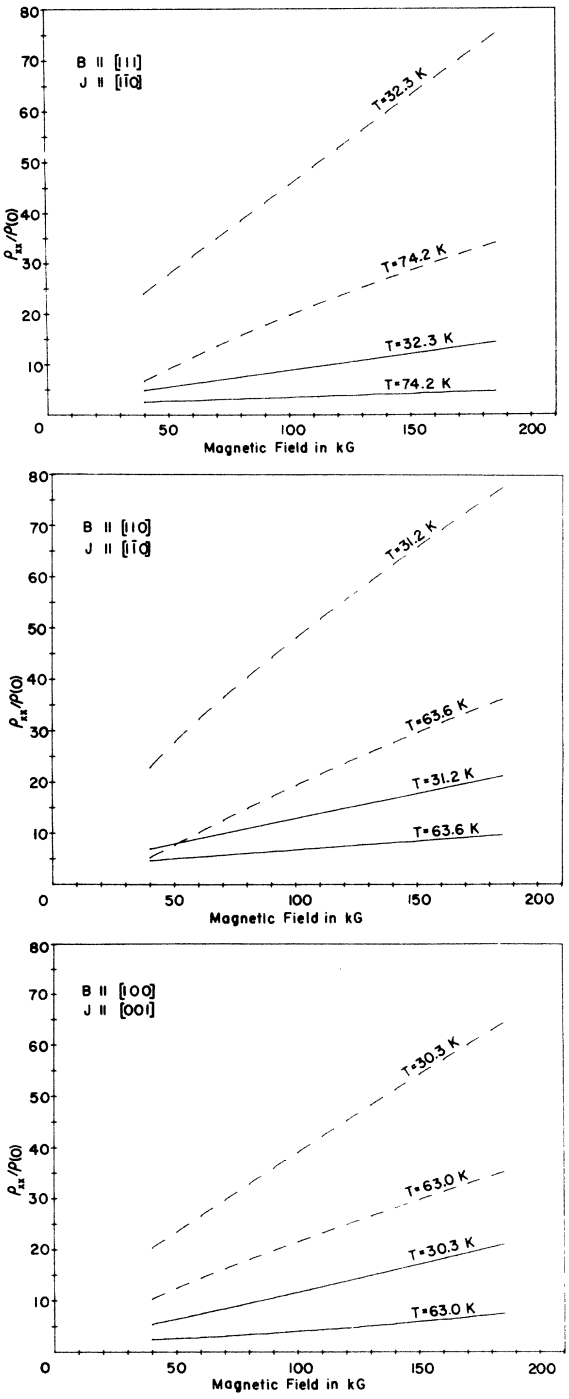

FIG. 1. Magnetoresistance ratio vs magnetic field. The solid curve are experimental and the dashed curves are what would be found theoretically if one set $\gamma = 0$.

In order to see the field and temperature depen-

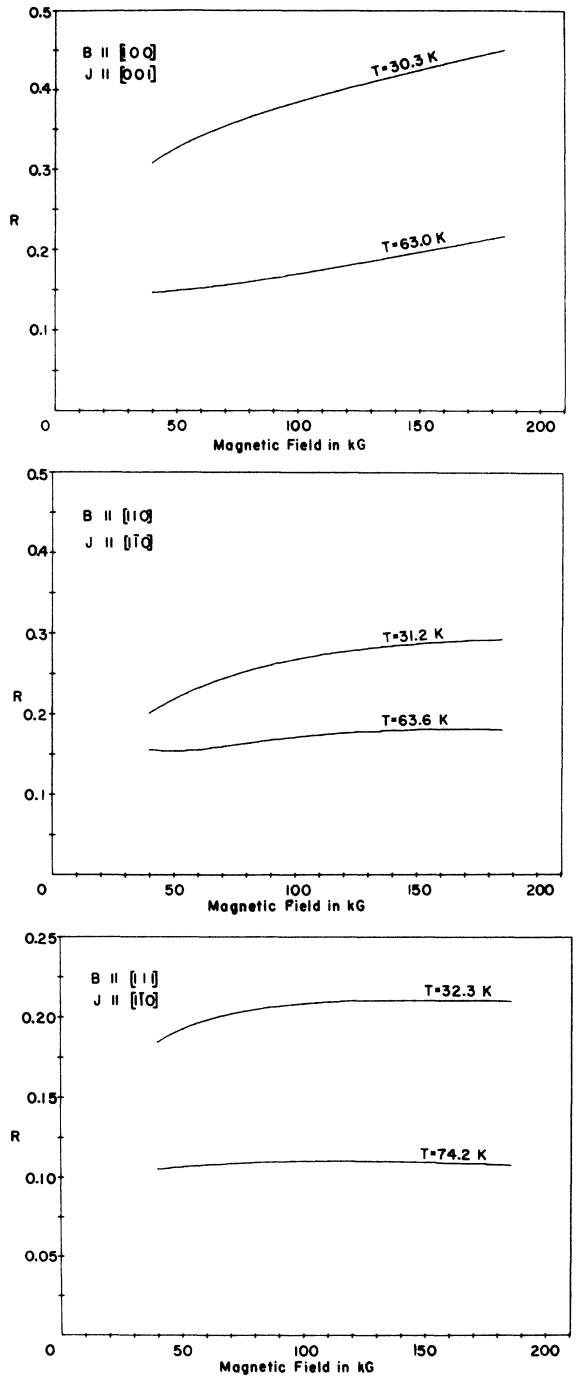

FIG. 2. Magnetic field vs ratios R that are necessary to obtain agreement between theory and experiment.

dences of $\langle 1/\tau_I^e \rangle_{av}$ of Eq. (3.33), $\langle 1/\tau_{nk} \rangle_{av}$ was calculated and multiplied by R. This assumes that $R_e \approx R$, i.e., for the range of $\vec{q}$ important here, it is assumed that there is no other scattering mechanism for phonons comparable to conduction-electron–phonon scattering. The resulting $\langle 1/\tau_I^e \rangle_{av}$ for each case of Figs. 1 and 2 is plotted in Fig. 3.

Calculations were also carried out assuming elastic scattering in order to see the effects of inelasticity. The dashed curves of Fig. 1 were found to be about twice as high for elastic scattering while the R's of Fig. 2 were about half as large. However, the curves of Fig. 3 remained almost unchanged. This is because the magnetoresistance

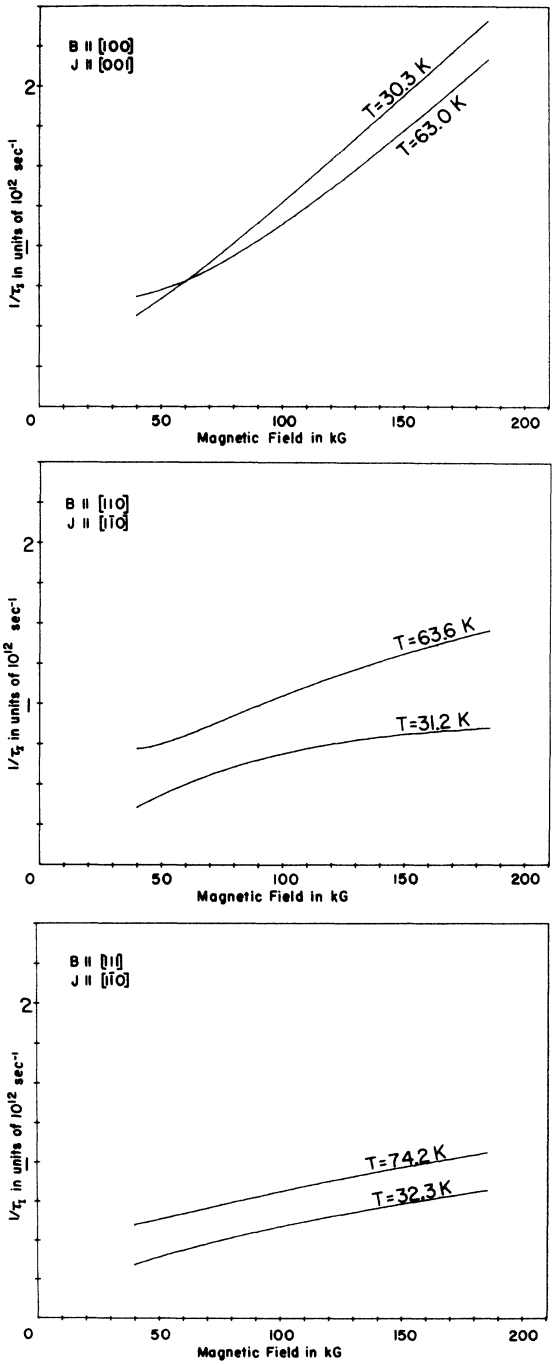

FIG. 3. Reciprocal of the secondary relaxation time for electrons corresponding to the R's of Fig. 2.

is proportional to both $\langle 1/\tau_{nk}\rangle_{av}$ and to R, since $(1-\gamma)$ is approximately equal to R for small R. Because R is proportional to the reciprocal of $\langle 1/\tau_{nk}\rangle_{av}$ these factors tend to cancel. Thus the experimental transverse resistance should be almost independent of $\langle 1/\tau_{nk}\rangle_{av}$ at large magnetic fields when acoustic-phonon scattering predominates. Therefore, while high-magnetic-field longitudinal magnetoresistance measurements[1] give information primarily about $\langle 1/\tau_{nk}\rangle_{av}$, high-field transverse magnetoresistance measurements primarily depend on secondary scattering mechanisms.

At low magnetic fields, one expects ionized impurity scattering to be the most important secondary scattering mechansim. Calculations to find $\langle 1/\tau_I^e\rangle_{av}$ for this mechanism were carried out. It was found that this scattering could account for the curves of Fig. 3 up to 50 or 60 kG. However, for large magnetic fields ionized impurity scattering is approximately proportional to B^{-2} and is more than an order of magnitude too low at fields around 200 kG. Thus other scattering mechanisms must be considered which are small at low magnetic fields and which increase as B increases.

One possibility is scattering with optical-phonon emission since spacing between different Landau levels and also between Landau levels and impurity levels increases with magnetic field. However, for the fields considered here none of the spacings between appreciably occupied levels and lower levels is yet equal to optical-phonon energies.

The most probable scattering mechanism appears to be through transitions to excited bound-impurity states by acoustic-phonon emission followed by transitions back to the conduction band with absorption of an acoustic phonon. Owing to shielding by conduction band electrons[22] relatively few bound-impurity states will exist for low magnetic fields. High magnetic fields give appreciably more bound states, increasing the transition probabilities. The overall transition rate is largely determined by that from the conduction band to impurity levels since the transitions back to the conduction band are to levels with a much greater energy density. Order-of-magnitude calculations were performed to find $\langle 1/\tau_I^e\rangle_{av}$ for transitions from the conduction band to an impurity level with a characteristic orbit size of about $L_z = 10^{-5}$ cm along the z axis and 10^{-6} cm for transverse directions. These lengths respectively correspond to a hydrogenlike impurity in its fifth or sixth excited level and to transverse size λ owing to the magnetic field. It was found that at 180 kG about 100 bound states in an energy range of 5×10^{-4} eV below the lowest Landau level are necessary to give the reciprocal relaxation times of Fig. 3. The energy 5×10^{-4} eV comes from the energy δ function occurring in transition probabilities and is the energy of an acoustic longitudinal phonon with a wave vector $\vec{q}$ of magnitude $1/\lambda$.

The number of bound states may be roughly estimated. If one assumes that the last bound states at zero magnetic field correspond to a hydrogen orbital quantum number of 5 or 6, then, as seen above, the transverse dimensions of the wave function at high fields is small compared to the longitudinal dimension. The wave function is approximately that of a one-dimensional hydrogen atom (taking effective mass and dielectric constant into account) times a transverse part due only to the magnetic field. This transverse part is characterized by quantum numbers n, specifying the Landau level, and l.[23] The energy will depend only slightly on l as long as the transverse dimensions are small compared with the longitudinal size L_z of the one-dimensional hydrogen-atom orbitals. The z component of angular momentum is $(n-l)\hbar$. For small n, the transverse dimensions are comparable to $l^{1/2}\lambda$. Therefore the number of bound states for a given hydrogenlike quantum number will be comparable to $l = (L_z/\lambda)^2 \simeq 100$ for $L_z \simeq 10^{-5}$ cm at 180 kG. Also, since the ground-state energy of the impurity is comparable to 10^{-2} eV, for hydrogen orbital quantum numbers around 5 or 6 these will be within less than 10^{-3} eV below the Landau levels. This meets the order-of-magnitude criterion of the preceding paragraph.

One may also consider magnetic field and temperature dependence of the relaxation time. In the calculation of $\langle 1/\tau_I^e\rangle_{av}$ the summation over phonon modes introduces a factor of B since the important range of both q_x and q_y is comparable to $1/\lambda$. Also, the number of wave functions that overlap with an impurity wave function in transverse directions is proportional to $\lambda^2 \sim B^{-1}$. Furthermore, the number of impurity bound states, by the argument above, is proportional to $(L_z/\lambda)^2 \sim B$. The energy δ function has only a slight B dependence. Hence one expects the reciprocal relaxation time to be approximately proportional to B for large fields.

Next let us consider temperature dependence. The number of phonons is proportional to T in the approximation of Eq. (3.22). Also, because of energy conservation only electrons within an energy interval comparable to the phonon energy, 5×10^{-4} eV, above the Landau level can make transitions to impurity bound state. Since the momentum distribution is one dimensional in the conduction band, this leads to a factor of $T^{-1/2}$. Finally, the number of bound states depends on temperature; as the temperature is lowered, the shielding due to conduction electrons is less[22] since classically the average electron energy is lower and thus the fractional change in velocity on entering the field of an impurity atom is greater, causing conduction electrons to spend less time near the impurity for lower temperature. Without more detailed calculations

all one can say is that the reciprocal relaxation time increases less rapidly than $T^{1/2}$ or else decreases with increasing T.

For the magnetic fields and temperature considered here, one can not test these qualitative ideas for the magnetic field in the [110] and [111] directions since the shift of electrons from low-mass to high-mass energy ellipsoids is not complete and several relaxation times are present. However, for the [100] direction all ellipsoids make the same angle relative to the magnetic field and also almost all the electrons are in the lowest Landau level at 180 kG. Thus, the arguments above should apply. The curves in Fig. 3 for the [100] direction do agree with the field and temperature dependences discussed above.

It should be noted that while it has been assumed that $R \approx R_e$, phonon scattering is involved in the mechanism just discussed and thus R_p is not zero. However, if it is assumed that phonon and electron scattering are related, the phonon relaxation times are proportional to those for the electrons for those scatterings which involve phonons and thus R_e and R_p should be comparable and have similar B and T dependences for high magnetic fields where ionized impurity scattering is unimportant.

Both scattering mechanisms considered depend on impurities and should decrease with decreasing impurity concentration. The ionized impurity scattering is proportional to the number of impurities. However, the scattering due to transitions to impurity states should vary less rapidly than the number of impurities since the shielding is less due to conduction electrons for a smaller concentration of donor impurities. Thus, one would expect that experimental curves for a small number of impurities would be below those of Fig. 1 with possibly a plateau or dip forming around 40 or 50 kG where the two scattering mechanisms are comparable. This behavior is seen in the experiments of Babich *et al.*[7]

In conclusion, it is seen that a nonequilibrium phonon distribution can greatly alter the transverse magnetoresistance. It is felt that the secondary scattering mechanisms discussed here involving impurities are the important ones for the range of parameters considered. More detailed calculations of relaxation times due to impurities are necessary to definitely establish this. It is probably not useful to carefully take into account both longitudinal and transverse phonons[7] since the transverse magnetoresistance is rather insensitive to direct electron-phonon scattering.

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