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Electronic Contribution to Magneto-Thermoelectric Power in Many-Valley Model of n-Ge

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ELECTRONIC CONTRIBUTION TO MAGNETO-THERMOELECTRIC POWER IN MANY-VALLEY MODEL OF n-Ge

by

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TABLE OF CONTENTS

CHAPTER I

INTRODUCTION

Investigation of the charge and the heat transport is one of the basic methods for the study of the characteristic parameters of electrons and phonons in solids. Earlier theoretical transport studies have been based on the use of the semiclassical Boltzman transport equation, where an assumption is made regarding the existence of a relaxation time.[1] But this equation has several shortcomings. A review article by Dresden[2] does an excellent job of explaining the limitations of the Boltzman equation, especially for problems involving a magnetic field where the quantum effects become quite important. In his conclusion, he strongly emphasizes the need of starting from more basic notions of statistical mechanics. In treating quantum-mechanical systems, it is necessary to deal with two types of uncertainties. The first type is due to the probabilistic nature of the wave-function, as is illustrated by the "Uncertainty Principle"; the second uncertainty occurs when one does not have sufficient information to find the quantum-mechanical state of the system. That second type can be handled by employing the density matrix formalism. An exposition of the use of the density matrix for magnetotransport problems has been given by Arora.[3]

The density matrix has been extensively used in literature for the study of electronic transport in a strong magnetic field.[4,5] These "quantum limit" calculations had the unpleasant drawback of a divergence difficulty, for which several cutoff mechanisms were suggested to achieve finite results.

Obviously, the results are sensitive to the cutoff used, and hence several conflicting results emerged. In spite of the large amount of theoretical and experimental work on magnetoresistance, there has not been much work to compare the theoretical analysis with the experimental works. This has been in part due to the belief that inhomogeneities play a larger role in magnetotransport phenomena.[6] The recent experiments of several workers[7,8] have indicated, however, that there is very little correlation between inhomogeneities and magnetotransport coefficients, especially for thermomagnetic effect.

Arora and co-workers[9,10,11] have investigated the linearization procedure used earlier.[4,5] They found that these theories involve essentially expansions in powers of $(\omega_c \tau)^{-1}$ with only the first-order terms retained. Here, ω_c is the cyclotron frequency and τ is the average momentum relaxation time. The divergence difficulties arise because the electrons making transitions to the bottom of Landau sub bands have relaxation times which are very small, thus violating the condition $\tau \omega_c \gg 1$ upon which the theories are based. It was suggested that this divergence could be eliminated by extending the scattering dynamics beyond the strict Born approximation.

Arora and Miller[9] have used the density matrix formalism to study the experimentally observed magnetoresistance on n-type Germanium where phonon-drag was also induced. The aims in this thesis are to present a theory based on these earlier works for electronic contribution to the thermoelectric power, and to perform numerical computations for comparison with the experimental data.

The phonon-drag contribution is not included in the present work.

Jay-Gerin[12] has calculated the contribution of electrons to the transverse thermoelectric power of a parabolic semiconductor with isotropic effective mass in the extreme quantum limit, when all the carriers in the conduction band are in the lowest Landau level. For the lowest-order approximation in the high-field limit, the thermoelectric power was found to be a monotonically increasing function of the magnetic field, independently of any electron scattering mechanism. Jay-Gerin's results are probably correct in the extreme quantum limit for a model where the relaxation time can be taken to be approximately equal to its value at the Fermi energy.

Demars et al[13] have performed some experiments on n-type GaSb at room temperature to study thermomagnetic effects predicted by the classical theoretical expression of Harman and Honing. They claim that the agreement between theory and experiment is good for magnetic fields up to 3.2 Wb/m^2. This may be due to the fact that quantum effects are not important at this value of the magnetic field, for GaSb.

Puri and Geballe[6] use Herring's π-approach to arrive at theoretical expressions (including both electron and phonon-drag contributions) for thermoelectric power in the quantum domain, for parabolic semiconductors with isotropic effective mass. They use these results to interpret their experimental observations on n-type Germanium. The effect of ellipsoidal energy surface was included in an average way. Hence the expression was not rigorous. n-type Germanium has a four-ellipsoidal band structure. Therefore, the effective mass is anisotropic and hence the theories for parabolic bands[6] cannot be applied directly. Moreover, due to the presence of quantization effects, the

semiclassical approach is not valid, especially at high magnetic fields. We, therefore, use the density matrix approach[9] to calculate thermomagnetic coefficients for an ellipsoidal energy surface.

The unperturbed wave function is given in Chapter II along with some useful matrix elements utilizing these functions. In Chapter III, the density matrix for the electron system is derived, assuming the phonon distribution to be in equilibrium, and treating the electric field as a perturbation. Using the electron-phonon scattering potential, the relaxation time is derived. The magnetotransport coefficients are derived and evaluated in Chapter IV, and the average values of the electric and the energy currents are found, with the use of the density matrix of Chapter III. The application of these results to n-type Ge and the comparison with the experimental measurement are made in Chapter V.

CHAPTER II

WAVE FUNCTIONS FOR THE ELECTRON

In the effective mass approximation, the unperturbed Hamiltonian for an electron in an anisotropic crystal in the presence of a magnetic field is:

$$\mathcal{H}_0 = \frac{1}{2m} \sum_{i,j} \alpha_{ij} \left(p_i + \frac{eA_i}{c}\right)\left(p_j + \frac{eA_j}{c}\right) \qquad \text{(II-1)}$$

where α_{ij}/m is the reciprocal mass tensor with $i,j = 1,2,3$ and A_i is a component of the vector potential. In the equation (II-1) the interaction between the electron and the scattering mechanism of the lattice vibration is neglected, because it is treated as a perturbation in Chapter III. For the special case of Germanium, the energy surfaces are ellipsoids of revolution with principal axes along the $\{111\}$ direction. Only one ellipsoid is considered in the intermediate calculation. When the final results are computed, the appropriate summation for the currents over four ellipsoids is made. If the axes of the coordinate system are chosen to coincide with the principal axes, with the z-axes along the longitudinal axis ("axis of symmetry") of the ellipsoid, then the α_{ij} forms a diagonal matrix with diagonal components:

$$(\alpha_{11})_0 = (\alpha_{22})_0 = \alpha_1 \quad \text{and} \quad (\alpha_{33})_0 = \alpha_3 \qquad \text{(II-2)}$$

and $\frac{m}{\alpha_1}, \frac{m}{\alpha_3}$ are the transverse and longitudinal masses, respectively, and $(\alpha_{ij})_0$ represents that α_{ij} is evaluated in the principal-axes frame. For an arbitrary choice of coordinates, α_{ij} will be more complicated. Since the ellipsoid is an ellipsoid of revolution, only the angle, θ,

between the magnetic field applied parallel to the z-axis on the longitudinal axis of the ellipsoid, is relevant. The original directions of the x and y axes can always be chosen such that θ is the result of merely a rotation around, say, the y axis. Such a rotation can be represented by the matrix:

$$\underline{\underline{R}} = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \qquad \text{(II-3)}$$

where the double bar indicates a tensor quantity. The diagonal matrix $\underline{\underline{\alpha}}$ transforms upon the θ rotation as:

$$\underline{\underline{\alpha}}' = \underline{\underline{R}}^{-1}\,\underline{\underline{\alpha}}\,\underline{\underline{R}} \qquad . \qquad \text{(II-4)}$$

Explicitly, one finds that in the rotated system $\underline{\underline{\alpha}}'$ can be represented by the matrix:

$$\underline{\underline{\alpha}}' = \begin{pmatrix} \alpha_1\cos^2\theta + \alpha_3\sin^2\theta & 0 & (\alpha_1-\alpha_3)\sin\theta\cos\theta \\ 0 & \alpha_2 & 0 \\ (\alpha_1-\alpha_3)\sin\theta\cos\theta & 0 & \alpha_1\sin^2\theta + \alpha_3\cos^2\theta \end{pmatrix}. \qquad \text{(II-5)}$$

In the presence of a uniform magnetic field with magnetic vector potential $\vec{A}=(0,Bx,0)$ in the Landau gauge, the Hamiltonian of equation (II-1) can be written as:

$$\mathcal{H}_0 = \frac{1}{2m}\left[\alpha_{11}P_x^2 + 2\alpha_{13}P_xP_z + \alpha_{22}(P_y+m\omega x)^2 + \alpha_{33}P_z^2\right] \qquad \text{(II-6)}$$

with $\omega = \frac{eB}{mc}$, the cyclotron frequency. From equation (II-6) it is clear that $\mathcal{H}_0$ commutes with both P_y, and P_z; therefore $\mathcal{H}_0$, P_y, P_z, can be diagonalized simultaneously. Putting in equation (II-6) the eigenvalues $\hbar k_y$, $\hbar k_z$ of P_y and P_z respectively, one obtains the following Schrodinger equation:

$$\frac{\hbar^2}{2m}\left[-\alpha_{11}\frac{\partial^2}{\partial x^2} - 2i\alpha_{13}k_z\frac{\partial}{\partial x} + \alpha_{22}\frac{m^2\omega^2}{\hbar^2}\left(x+\frac{\hbar k_y}{m\omega}\right)^2 + \alpha_{33}k_z^2\right]\phi_{nk}(x) =$$

$$E_{nk}\,\phi_{nk}(x)$$

where $\mathcal{E}_{nk}$ is the energy eigenvalue and $\vec{k} = (k_y, k_z)$.

We make the assumption

$$\phi_{nk}(x) = \phi_k(x) e^{\delta x} \tag{II-8}$$

where $\phi_{nk}(x)$ is a function of x and δ is a constant, that we substitute this solution in equation (II-7) and choose δ so that the coefficient of $\frac{\partial \phi_{nk}(x)}{\partial x}$ is zero:

$$\delta = -i \frac{\alpha_{13}}{\alpha_{11}} k_z \tag{II-9}$$

Then the function $\phi_k(x)$ satisfies the differential equation:

$$\left[-\frac{\alpha_{11}\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{\alpha_{22} m\omega^2}{2}\left(x + \frac{\hbar k_y}{m\omega}\right)^2\right]\phi_k(x) = \left[\mathcal{E}_{nk} - \frac{\alpha_1 \alpha_3}{2\alpha_{11} m}\hbar^2 k_z^2\right]\phi_k(x) \tag{II-10}$$

which has the same form as the Schrodinger equation for the harmonic oscillator, with the origin displaced by $\frac{\hbar k_y}{m\omega}$. The eigenvalue and eigenfunction of this equation are well known[15]:

$$\mathcal{E}_{nk} = (n + \tfrac{1}{2})\hbar\omega^* + \frac{\alpha_1^2 \hbar^2 k_z^2}{2m^*} \quad \text{for} \quad n = 0, 1, 2, 3, \ldots \tag{II-11}$$

with

$$\phi_k(x) = \left(\frac{\alpha}{\pi^{1/2} 2^n n!}\right)^{1/2} H_n[\alpha(x + \lambda^2 k_y)] e^{-\frac{1}{2}\alpha^2 (x + \lambda^2 k_y)^2} \tag{II-12}$$

where $H_n[\alpha(x+\lambda^2 k_y)]$ is a Hermite polynomial of order n, and

$$\omega^* = (\alpha_1 \alpha_{11})^{1/2} \omega \quad , \tag{II-13}$$

$$\lambda = \left(\frac{\hbar c}{eB}\right)^{1/2} \quad , \tag{II-14}$$

$$m^* = \frac{\alpha_{11} m}{\alpha_1 \alpha_3} \quad , \tag{II-15}$$

$$\alpha = \alpha_1^{1/4} / (\lambda \alpha_{11}^{1/4}) \tag{II-16}$$

The complete wave function of the Hamiltonian of equation (II-6) is then given by

$$\Phi_{nk}(\vec{r}) = \phi_n[\alpha(x+\lambda^2 k_y)]\, e^{-i\beta k_z x + i(k_y y + k_z z)} \qquad \text{(II-17)}$$

with

$$\beta = \alpha_{13}/\alpha_{11}$$

We shall also need, in the following, the matrix elements of between two energy states; we find that

$$\langle n;k'|e^{i\vec{q}\cdot\vec{r}}|n,k\rangle = \delta(k_y' - q_y - k_z)\,\delta(k_z' - q_z - k_z)\, J_{n'n}(q_x, k_y', k_y, k_z) \qquad \text{(II-18)}$$

where

$$J_{n'n}(q_x, k_y', k_y, k_z) = \int_{-\infty}^{\infty} \phi_{n'}[\alpha(x+\lambda^2 k_y)]\, e^{-i(q_x+\beta k_z)x}\, \phi_n[\alpha(x+\lambda^2 k_y)]\, dx \qquad \text{(II-19)}$$

The quantities $J_{n'n}$ have some useful properties[15] which make the treatment of scattering among different oscillator states treatable. First, $|J_{n'n}(q_x, k_y', k_y, k_z)|^2$ is a function of $(q_x^2 + q_y^2)$ only, as can be proved with the use of the generating function for the $\phi_n(x)$; it is actually a polynomial in $(q_x^2 + q_y^2)$ multiplied by

$$\exp\left[-\left(\frac{\hbar^2}{2m}\right)(q_x^2 + q_y^2)/\hbar\omega\right]$$

Secondly, for all n and n'

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |J_{n'n}(\pm q_x, \pm q_y + k_y, k_y, k_z)|^2\, dq_x\, dq_y = \frac{2\pi}{\lambda^2} \qquad \text{(II-20)}$$

This is proved as follows:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |J_{n'n}|^2\, dq_x\, dq_y = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dq_x\, dq_y \int_{-\infty}^{\infty} dx\, \phi_{n'}[\alpha(x+k_y\lambda^2)]\, e^{-i(q_x+\beta q_z)x}\, \phi_n[\alpha(x+\lambda^2 k_y)]$$
$$\times \int_{-\infty}^{\infty} dy\, \phi_{n'}[\alpha(y+\lambda^2 k_y')]\, e^{i(q_x+\beta q_z)y}\, \phi_n[\alpha(y+\lambda^2 k_y)]\,. \qquad \text{(II-21)}$$

$$= \iiint dq_{fy}\, dx\, dy\, \phi_{n'}[\alpha(y+\lambda^2 k_y')]\, \phi_n[\alpha(x+\lambda^2 k_y)]\, \phi_{n'}[\alpha(y+\lambda^2 k_y')]$$

$$\times \phi_n[\alpha(y+\lambda^2 k_y)]\, e^{i\beta q_{fy}(y-x)} \int_{-\infty}^{\infty} dq_{fx}\, e^{iq_x(y-x)} \qquad \text{(II-22)}$$

However

$$\int_{-\infty}^{\infty} e^{iq_x(y-x)}\, dq_x = 2\pi\, \delta(y-x) \qquad \text{(II-23)}$$

Therefore we have, after an integration over x,

$$\iint_{-\infty}^{\infty} |J_{n'n}|^2\, dq_x\, dq_{fy} = 2\pi \int_{-\infty}^{\infty} \phi_n^2[\alpha(y+\lambda^2 k_y)]\, dy \int_{-\infty}^{\infty} dq_{fy}\, \phi_{n'}^2[\alpha(y+\lambda^2 k_y')]; \qquad \text{(II-24)}$$

However $s = \lambda^2 k_y'' = \lambda^2(k_y + q_{fy})$, where k_y = constant, and thus, $dq_{fy} = \frac{ds}{\lambda^2}$.

Therefore

$$\iint_{-\infty}^{\infty} |J_{n'n}|^2\, dq_{fy}\, dq_{fx} = \frac{2\pi}{\lambda^2} \int_{-\infty}^{\infty} \phi_n^2[\alpha(y+\lambda^2 k_y)]\, dy \int_{-\infty}^{\infty} ds\, \phi_{n'}^2[\alpha(y+s)] \qquad \text{(II-25)}$$

Since the functions are normalized to unity, one obtains finally

$$\iint_{-\infty}^{\infty} |J_{n'n}|^2\, dq_x\, dq_{fy} = \frac{2\pi}{\lambda^2} \qquad \text{(II-26)}$$

CHAPTER III

DENSITY MATRIX FOR AN ELECTRON IN A CRYSTAL

In the absence of a perturbation, the quantum mechanical state of an electron is well represented by an eigenfunction of the type (II-17). As discussed in the introduction, when the perturbation is present, we do not know precisely the state of the system, necessitating an expansion of the wave function ψ^i of an electron (say the ith electron) in terms of the orthonormal set of equation (II-17):

$$\psi^i(t) = \sum_\alpha a^i_\alpha(t)\,|\alpha\rangle \qquad \text{(III-1)}$$

where $|\alpha\rangle$ is the eigenfunction $\phi_{n\bar{k}}(\bar{r})$ in the familiar Dirae notation; α stands for the set of quantum numbers (n, k_y, k_z) .

Let f be some physical quantity pertaining to the system considered. Then the expectation value of this quantity in the state $\psi^i(t)$ is given by:

$$f^i = \langle \psi^i | f | \psi^i \rangle = \sum_\alpha \sum_{\alpha'} a^{i*}_{\alpha'}(t)\, a^i_\alpha(t) \langle \alpha' | f | \alpha \rangle \,. \qquad \text{(III-2)}$$

An ensemble average for the electrons in the system, then, can be described by:

$$\langle f \rangle = \frac{1}{N} \sum_i f^i = \frac{1}{N} \sum_i^N \sum_\alpha \sum_{\alpha'} \langle \alpha' | f | \alpha \rangle\, a^{i*}_{\alpha'}(t)\, a^i_\alpha(t), \qquad \text{(III-3)}$$

where N is the number of free electrons in the crystal.

If we define

$$\frac{1}{N} \sum a^i_\alpha(t)\, a^{i*}_{\alpha'}(t) \equiv \langle \alpha | \rho | \alpha' \rangle, \qquad \text{(III-4)}$$

equation (III-3) can be written as:

$$\langle f \rangle = \sum_\alpha \sum_{\alpha'} \langle \alpha | \rho | \alpha' \rangle \langle \alpha' | f | \alpha \rangle = Tr(\rho f) \qquad \text{(III-5)}$$

where tr stands for the sum of the diagonal elements. Let us now suppose that the system is closed, or became so at some instant. Then we can derive an equation giving the change in the density matrix with time. Using the equation (III-1) and the orthonormality property of the $|\alpha\rangle$'s, we can write an equation for the time-dependence of the a_α's : if $\mathcal{H}$ is the full Hamiltonian describing the electron,

$$i\hbar \frac{d}{dt} a^*_\alpha(t) = \sum_{\alpha'} \langle\alpha|\mathcal{H}|\alpha'\rangle a^*_{\alpha'}(t); \qquad \text{(III-6)}$$

Using this time dependence in equation (III-4), we obtain Liouville's equation for the density matrix:

$$i\hbar \frac{\partial \rho}{\partial t} = [\mathcal{H}, \rho]. \qquad \text{(III-7)}$$

Our purpose is to find the steady state ρ at $t=0$ when

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}', \qquad \text{(III-8)}$$

and

$$\mathcal{H}' = V + P, \qquad \text{(III-9)}$$

where V is the electron-phonon interaction potential and P is the electron-external electric field interaction

$$P = e\,\vec{\mathcal{E}}\cdot\vec{r}\,. \qquad \text{(III-10)}$$

The total density matrix ρ_T for the perturbed system in the presence of an electric field can be written as a sum of an equilibrium part ρ_0, independent of an electric field, and ρ', depending upon the electric field:

$$\rho_T = \rho_0 + \rho'(t). \qquad \text{(III-11)}$$

In the time-development of the system, we assume the perturbation $\mathcal{H}'$ to be absent at time $t = -\infty$, when it is turned on slowly according to

$$\mathcal{H}(t) = \mathcal{H}' e^{st}, \tag{III-12}$$

where s is a small positive number $(s \rightarrow 0^+)$. The non-equilibrium part of the density matrix $\rho'(t)$ will follow a similar time dependence:

$$\rho'(t) = \rho' e^{st}, \tag{III-13}$$

We want to study the steady-state behavior of the system at time $t=0$, which could be obtained by taking the limit $s \rightarrow 0^+$, when $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}'$ and $\rho_T = \rho_0 + \rho'$. Substituting the time dependence of $\mathcal{H}'(t)$ and $\rho'(t)$ in Liouville's equation (III-7), we have:

$$i\hbar s \rho' e^{st} = [\mathcal{H}_0, \rho_0] + [\mathcal{H}_0, \rho' e^{st}] + [\mathcal{H}' e^{st}, \rho_0] + [\mathcal{H}' e^{st}, \rho' e^{st}] \tag{III-14}$$

Since ρ_0 is diagonal in $\mathcal{H}_0$-representation, the part $[\rho_0, \mathcal{H}_0]$ equals zero.

Taking matrix elements of equation (III-14) between state $|\alpha'\rangle$ and $|\alpha\rangle$ one obtains the coupled equation for matrix elements of ρ':

$$(\varepsilon_{\alpha'\alpha} - i\hbar s)\langle\alpha'|\rho'|\alpha\rangle = \langle\alpha'|[\rho_0 F]|\alpha\rangle + f_{\alpha'\alpha}\langle\alpha'|V|\alpha\rangle + \langle\alpha'|[\rho', \mathcal{H}']|\alpha\rangle e^{st} \tag{III-15}$$

where $$\varepsilon_{\alpha'\alpha} = \varepsilon_{\alpha'} - \varepsilon_{\alpha}, \tag{III-16}$$

and $$f_{\alpha'\alpha} = f_{\alpha'} - f_{\alpha}. \tag{III-17}$$

To decouple these equations, usually a linearization procedure is adopted.[4] According to this procedure, the last term involving $[\rho', \mathcal{H}']$ is neglected on the grounds that this involves higher-order terms. This allows us to solve $\langle\alpha'|\rho'|\alpha\rangle$ from equation (III-15) in terms of the first-order terms in $\mathcal{H}'$. This first-order expression of $\langle\alpha'|\rho'|\alpha\rangle$ is then used to generate second- and higher-order terms.

This procedure is equivalent to generation of a series in terms of $(\omega^* \tau)^{-1}$, of which only the first two terms are to be kept under the assumption of a strong magnetic field $(\omega^* \gg \frac{1}{\tau})$. But higher-order terms in the series may also become important for-those electrons making transitions to the bottom of conduction bands $(k_z = 0)$, thereby invalidating the expansion. This is avoided by solving equation (III-15) exactly:

$$\langle \alpha' | \rho' | \alpha \rangle = \frac{\langle \alpha' | [P_0, F] | \alpha \rangle + f_{\alpha\alpha} \langle \alpha' | V | \alpha \rangle + \langle \alpha' | [P', \mathcal{H}'] | \alpha \rangle e^{s\epsilon}}{\epsilon_{\alpha'\alpha} - i\hbar s}, \tag{III-18}$$

This exact expression is then used in the last term of equation (III-15) to get:

$$(\epsilon_{\alpha'\alpha} - i\hbar s) \langle \alpha' | \rho' | \alpha \rangle = \langle \alpha' | [P_0, F] | \alpha \rangle + f_{\alpha'\alpha} \langle \alpha' | V | \alpha \rangle$$

$$+ \sum_{\alpha''} \frac{\langle \alpha' | [P_0, F] | \alpha'' \rangle + f_{\alpha'\alpha''} \langle \alpha' | V | \alpha'' \rangle + \langle \alpha' | [P', \mathcal{H}'] | \alpha'' \rangle e^{s\epsilon}}{\epsilon_{\alpha'\alpha''} - i\hbar s} \langle \alpha'' | \mathcal{H}' | \alpha \rangle$$

$$- \sum_{\alpha''} \langle \alpha' | \mathcal{H}' | \alpha'' \rangle \cdot \frac{\langle \alpha'' | [P_0, F] | \alpha \rangle + f_{\alpha''\alpha} \langle \alpha'' | V | \alpha \rangle + \langle \alpha'' | [P', \mathcal{H}'] | \alpha \rangle e^{s\epsilon} \cdot e^{s\epsilon}}{\epsilon_{\alpha''\alpha} - i\hbar s} \tag{III-19}$$

At this stage, we use approximations to decouple this equation for matrix elements of ρ'. First, since we are interested in the ohmic currents (which are linear in an electric field), we neglect the $[P', F]$- term, which involves a higher order in the electric field. Now we take the ensemble average over the scatters. The first-order term in V will then drop out because of random phases. Second-order terms in V which cannot be reduced to the form of $|\langle \alpha | V | \alpha'' \rangle|^2$ will also drop out. Now, we take the limit $s \to 0$ and use the identity

$$\lim_{s \to 0} \frac{1}{x - is} = P\left(\frac{1}{x}\right) + i\pi\delta(x)$$

where $\mathcal{P}$ indicates the principal part. In the irreversible behavior of the current, the principal-part term will not contribute to the current, when the elastic scattering assumption is made.[16]

Finally, we make use of a property of the density matrix due to spatial invariance, described by Fano[17], according to which all elements of ρ which are non-diagonal in $\bar{k}$ -space ($k'_y \neq k_y$ and $k'_z \neq k_z$) are zero. This simplifies equation (III-17) to the form:

$$\varepsilon_{\alpha'\alpha}\langle\alpha'|\rho'|\alpha\rangle = \langle\alpha'|[\rho_0, F]|\alpha\rangle + \langle\alpha'|\rho'|\alpha\rangle \frac{i\hbar}{\tau_{\alpha'\alpha}} \quad , \tag{III-19}$$

where $$\frac{1}{\tau_{\alpha'\alpha}} = \frac{1}{2}\frac{1}{\tau_\alpha} + \frac{1}{2}\frac{1}{\tau_{\alpha'}} \quad , \tag{III-20}$$

with $$\frac{1}{\tau_\alpha} = \frac{2\pi}{\hbar}\sum_{\alpha'}\left|\langle\alpha|V|\alpha'\rangle\right|^2 \delta(\varepsilon_{\alpha\alpha'} \pm \hbar\omega_q) \, . \tag{III-21}$$

Here $\hbar\omega_q$ is the energy of an acoustic phonon of wave vector q and angular frequency ω_q, and the ($\pm$) in the parentheses of equation (III-21) stands for emission (-) and absorption (+) of a phonon.

Equation (III-19) now can be solved for the matrix element of ρ':

$$\langle\alpha'|\rho'|\alpha\rangle = \frac{\langle\alpha'|[\rho_0, F]|\alpha\rangle}{\varepsilon_{\alpha'\alpha} - \frac{i\hbar}{\tau_{\alpha'\alpha}}} \quad . \tag{III-22}$$

Equation (III-22) has a Breit-Wigner type of collision broadening built into it, in the denominator. The absence of this collision broadening was actually the cause of the divergence in earlier works[4,5]. Some authors[18] have artificially added a collision term of the form $\frac{\rho_0 - \rho}{\tau}$ to Liouville's equation (III-7). Arora's theory, on the other hand, incorporates Breit-Wigner broadening in a natural way.

The Relaxation Time for Acoustic-Phonon Scattering

For the electron-lattice interaction potential V, we shall take, as was done by Argyres and Adams,[19] an expression

$$V = E_1 \bar{\nabla} U(\bar{r}) \tag{III-23}$$

where the function, $U(\bar{r})$ describes the displacement of the atoms due to the lattice vibrations, and E_1 is the deformation potential constant. Expanding the lattice displacement in terms of the normal modes, one finds:

$$V = i E_1 \left(\frac{\hbar}{\rho_c \omega_q}\right)^{1/2} \sum Q_{\bar{q}} \, q \, e^{i \bar{q} \cdot \bar{r}} \tag{III-24}$$

where $\bar{q}$ is the wave vector of one of the normal mode phonons, $Q_{\bar{q}}$ is the annihilation operator, and ρ_c is the crystal density. Substituting equation (III-24) in equation (III-21) we get:

$$\frac{1}{\tau_\kappa} = \frac{2\pi}{\hbar} \frac{\hbar E_1^2}{\rho_c u_e} \sum_{\alpha'} \sum_{q} \left| \langle \alpha' | e^{i \bar{q} \cdot \bar{r}} | \alpha \rangle \right| q \left[(N_q \, \delta(\varepsilon_{\alpha\alpha'} + \hbar\omega_q) + (N_q + 1) \, \delta(\varepsilon_{\alpha\alpha'} - \hbar\omega_q) \right] . \tag{III-25}$$

Here u_e is the longitudinal sound velocity, N_q is the number of phonons with the wave vector $\bar{q}$ and $\omega_{\bar{q}}$ is the angular frequency of the phonon $\bar{q}$, usually taken to be $u_e q$. For a semiconductor such as Germanium, in the temperature above 20°K, the expression for N_q, which is the Bose-Einstein distribution function, can be approximated as:

$$N_q \simeq N_q + 1 = \frac{KT}{\hbar \omega_q} .$$

The equation (III-25) then simplifies to:

$$\frac{1}{\tau} = A \sum_{\alpha'} \sum_{q} \left| \langle \alpha' | e^{i \bar{q} \cdot \bar{r}} | \alpha \rangle \right|^2 \left[\delta(\varepsilon_{\alpha\alpha'} + \hbar\omega_q) + \delta(\varepsilon_{\alpha\alpha'} - \hbar\omega_q) \right] \tag{III-26}$$

with $$A = \frac{2\pi E_1^2 kT}{\hbar \rho U_\ell^2} \qquad \text{(III-27)}$$

Some simplifications are necessary in order to evaluate this summation. Following Arora[20] we can use, for $\hbar\omega_q$, the average phonon energy,

$$\langle \hbar\omega_q \rangle = \nu_p \frac{\hbar U_\ell}{\lambda} \qquad \text{(III-28)}$$

where ν_p is a parameter which is zero for elastic scattering and describes the extent of inelasticity of the collision, and λ is the radius of the cyclotron orbit in a magnetic field. Using equation (II-18) and this approximation, equation (III-26) takes the form:

$$\frac{1}{\tau} = A \sum_{\alpha'} \delta\left(\varepsilon_{\alpha'\alpha} + \nu_p \frac{\hbar U_\ell}{\lambda}\right) \sum_{q_x q_y} \left| J_{n'n}(q_x, k_y', k_y, k_z) \right|^2 + A \sum_{\alpha'} \delta\left(\varepsilon_{\alpha'\alpha} - \nu_p \frac{\hbar U_\ell}{\lambda}\right) \sum_{q_x q_y} \left| J_{n'n}(q_x, k_y', k_y, k_z) \right|^2 , \qquad \text{(III-29)}$$

and using equation (II-26) one obtains:

$$\frac{1}{\tau} = \frac{2\pi A}{\lambda^2} \sum_{\alpha'} \delta\left(\varepsilon_{\alpha\alpha'} + \nu_p \frac{\hbar U_\ell}{\lambda}\right) + \frac{2\pi A}{\lambda^2} \sum_{\alpha'} \delta\left(\varepsilon_{\alpha\alpha'} - \nu_p \frac{\hbar U_\ell}{\lambda}\right) . \qquad \text{(III-30)}$$

Converting the summation over k_z' into an integration, one finds:

$$\frac{1}{\tau} = \frac{A}{(2\pi\lambda)^2} \sum_{n'} \left\{ \int_{-\infty}^{\infty} dk_z' \, \delta\left(\varepsilon_{\alpha\alpha'} + \nu_p \frac{\hbar U_\ell}{\lambda}\right) + \int_{-\infty}^{\infty} dk_z' \, \delta\left(\varepsilon_{\alpha\alpha'} - \nu_p \frac{\hbar U_\ell}{\lambda}\right) \right\} . \qquad \text{(III-31)}$$

Using equation (II-11) to convert the integration over k_z' to an integration over $\varepsilon_{\alpha'}$ one finally obtains:

$$\frac{1}{\tau_\alpha} = \frac{A}{(2\pi\lambda)^2} \left(\frac{2m^*}{\hbar^2}\right)^{1/2} \sum_{n'}{}' \left[\varepsilon_\alpha - (n' + \tfrac{1}{2})\hbar\omega^* + \nu_p \frac{\hbar U_\ell}{\lambda}\right]^{-1/2} + \frac{A}{(2\pi\lambda)^2} \left(\frac{2m^*}{\hbar^2}\right)^{1/2} \sum_{n'}{}' \left[\varepsilon_\alpha - (n' + \tfrac{1}{2})\hbar\omega^* - \nu_p \frac{\hbar U_\ell}{\lambda}\right]^{-1/2} . \qquad \text{(III-32)}$$

The prime on the summation means that n' goes from zero to the largest integer n' for which $\varepsilon_\alpha - (n' + \frac{1}{2})\hbar\omega^* - \nu_p \frac{\hbar U_\ell}{\lambda} \geq 0$.

CHAPTER IV

MAGNETOTRANSPORT COEFFICIENTS

The theory of magnetotransport coefficients, as is well known, reduces to calculations of the components of the thermomagnetic tensors $\underline{\beta}(H), \underline{\varrho}(H), \underline{\gamma}(H)$ and $\underline{\chi}(H)$ defined by the relations:[10]

$$\bar{J} = \underline{\sigma} \cdot \bar{E}^* - \underline{\beta} \cdot \bar{\nabla} T \,, \tag{IV-1}$$

$$\bar{P} = \bar{W} + \zeta_f e^{-1} \bar{J} = \underline{\gamma} \cdot \bar{E}^* - \underline{\chi} \cdot \bar{\nabla} T \,. \tag{IV-2}$$

Here $\bar{J}$ is the electric current density, $\bar{W}$ is the total energy flux (taking the electrostatic energy into account), $\underline{\sigma}(H)$ is the electrical conductivity, $\underline{\chi}(H)$ is the thermal conductivity in the magnetic field $\bar{B}$, T is the temperature, $\bar{E}^*$ is a sum of the applied field and the field generated by the electrons because of an inhomogeneous temperature and electron distribution:

$$\bar{E}^* = \bar{E} + e^{-1} \bar{\nabla} \zeta_f(\bar{B}, n_e, T) \,, \tag{IV-3}$$

and ζ_f is the Fermi energy.

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

$$\bar{E}^* = \underline{Q} \cdot \bar{\nabla} T \tag{IV-4}$$

with the subsidiary condition $\bar{J}=0$. The absolute Peltier coefficient $\underline{\Pi}$ is defined by:

$$\bar{P} = \underline{\Pi} \cdot \bar{J} \tag{IV-5}$$

with the subsidiary condition $\bar{\nabla} T = 0$. The Seebeck and Peltier coefficients are connected by the Kelvin relation:[5]

$$\pi_{ij}(\vec{B}) = T Q_{ij}(-\vec{B}) \cdot \qquad \text{(IV-6)}$$

Equations (IV-1) and (IV-2), together with (IV-4) and (IV-5), show that:

$$\underline{\beta} = \underline{\sigma} \cdot \underline{Q} \cdot \qquad \text{(IV-7)}$$

$$\underline{\gamma} = \underline{\pi} \cdot \underline{\sigma} \cdot \qquad \text{(IV-8)}$$

The Kelvin relation (IV-6), together with the Onsager relation:

$$L_{ij}(\vec{B}) = L_{ij}(-\vec{B}) \qquad \text{(IV-9)}$$

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

$$\underline{\gamma} = T \underline{\rho} \cdot \underline{\beta} \cdot \underline{\sigma} \qquad \text{(IV-10)}$$

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

From equations (IV-10) and (IV-7):

$$\underline{Q} = \frac{1}{T} \underline{\gamma} \cdot \underline{\sigma}^{-1} \cdot \qquad \text{(IV-11)}$$

The tensor appearing in the definition of $\underline{Q}$ and the tensor $\underline{\sigma}$ can be determined by computing the electric and energy currents.

The operator for the energy current which is provided by the conduction electrons is:[10]

$$\hat{\vec{F}} = \frac{1}{2}\left[(\mathcal{H}_0 - \zeta)\hat{\vec{v}} + \hat{\vec{v}}(\mathcal{H}_0 - \zeta)\right] , \qquad \text{(IV-12)}$$

and the density operator for electric current is:

$$\hat{\vec{J}} = -e\hat{\vec{v}} \cdot$$

Here $\mathcal{H}_0$ is the Hamiltonian (equation II-1) and $\hat{\vec{v}}$ the velocity operator. The eigenfunctions of $\mathcal{H}_0$ are given by equation (II-17) and the eigen-

values by equation (II-11); the matrix elements of the velocity components in these representations are:

$$\langle \alpha' | \hat{v}_x | \alpha \rangle = \alpha_{11} \frac{ik}{m\sqrt{2}} \left(\frac{m}{\hbar^2 \alpha_{11}} \right)^{1/2} \left\{ (n+1)^{1/2} \delta_{n',n+1} - n^{1/2} \delta_{n',n-1} \right\} \delta_{k',k} \quad , \tag{IV-14}$$

$$\langle \alpha' | \hat{v}_y | \alpha \rangle = (\alpha_{11} \alpha_{22})^{1/2} \frac{k}{m\sqrt{2}} \left(\frac{m}{\hbar^2 \alpha_{11}} \right)^{1/2} \left\{ (n+1)^{1/2} \delta_{n',n+1} + n^{1/2} \delta_{n',n-1} \right\} \delta_{k',k} \quad , \tag{IV-15}$$

$$\langle \alpha' | \hat{v}_z | \alpha \rangle = \frac{\alpha_{13}}{m} \left(\frac{m}{\hbar^2 \alpha_{11}} \right)^{1/2} \hbar k_z \delta_{n'n} \delta_{k'k} + \frac{\alpha_{13}}{\alpha_{11}} \langle \alpha' | \hat{v}_x | \alpha \rangle \quad . \tag{IV-16}$$

Here $k = (k_y, k_z)$ is a two-dimensional vector.

The electric and energy currents are determined by use of the denisty matrix ρ from the statistical mechanical prescriptions

$$\bar{J} = \mathrm{Tr}(\rho \hat{J}) \quad , \tag{IV-17}$$

$$\bar{F} = \mathrm{Tr}(\rho \hat{F}) \quad , \tag{IV-18}$$

then

$$\bar{J} = \sum_{\alpha} \langle \alpha | \rho \hat{J} | \alpha \rangle = \sum_{\alpha} \sum_{\alpha'} \langle \alpha | \rho | \alpha' \rangle \langle \alpha' | \hat{J} | \alpha \rangle \tag{IV-19}$$

$$\begin{aligned} E &= \frac{1}{2} \sum_{\alpha} \langle \alpha | \rho \hat{v} (\vec{r}_0 - \vec{r}') | \alpha \rangle + \frac{1}{2} \sum_{\alpha} \langle \alpha | \rho (\vec{r}_0 - \vec{r}') \hat{v} | \alpha \rangle \\ &= \frac{1}{2} \sum_{\alpha} \sum_{\alpha'} \sum_{\alpha''} \langle \alpha | \rho | \alpha' \rangle \langle \alpha'' | V | \alpha \rangle \varepsilon_{\alpha''} \delta_{\alpha' \alpha''} \quad , \\ &\quad + \frac{1}{2} \sum_{\alpha} \sum_{\alpha'} \sum_{\alpha''} \langle \alpha | \rho | \alpha' \rangle \langle \alpha' | V | \alpha \rangle \varepsilon_{\alpha} \delta_{\alpha'' \alpha} - \frac{d}{e} \sum_{\alpha} \langle \alpha | \rho \hat{\bar{J}} | \alpha \rangle \end{aligned} \tag{IV-20}$$

Here $\langle \alpha | \rho | \alpha' \rangle$, $\langle \alpha | \rho | \alpha'' \rangle$ are given by equation (III-22) using equations (IV-14, 15, 16, 19) and (III-22) by defining:

$$\sigma_1 = \frac{e^2}{m} \alpha_{11} \sum_{\alpha} f_{\omega_1, \alpha} (n+1) \frac{1/\tau_{\omega_1, \alpha}}{\omega^2 + 1/\tau^2_{\omega_1, \alpha}} \quad , \tag{IV-21}$$

$$\sigma_2 = \sqrt{\sigma_{\alpha_{11}}} \frac{e^2}{m} \sum_{\alpha} f_{\omega_1, \alpha} (n+1) \frac{\omega^2}{\omega^2 + 1/\tau^2_{\omega_1, \alpha}} \quad , \tag{IV-22}$$

$$\sigma_3 = \frac{e^2}{m^2} \left(\frac{m \alpha_{13}^2}{\hbar^2 \alpha_{11}} \right) \sum_{\alpha} (\hbar k_z)^2 f_{\omega_1 \alpha} \tau_{\omega_1 \alpha} \quad , \tag{IV-23}$$

one finds the complete conductivity tensor as:

$$\underline{\underline{\sigma}} = \begin{pmatrix} \sigma_1 & -\sigma_2 & -\frac{\alpha_{13}}{\alpha_{11}}\sigma_1 \\ \sigma_2 & \frac{\alpha_1}{\alpha_{11}}\sigma_1 & -\frac{\alpha_{13}}{\alpha_{11}}\sigma_2 \\ \frac{\alpha_{13}}{\alpha_{11}}\sigma_1 & \frac{\alpha_{13}}{\alpha_{11}}\sigma_2 & \sigma_1\frac{\alpha_{12}}{\alpha_{11}} + \sigma_3 \end{pmatrix}. \qquad \text{(IV-24)}$$

By using equations (IV-14, 15, 16, 20) and (III-22) and defining:

$$\gamma_1 = -\frac{e}{m}\alpha_n \sum_{\alpha} f_{\alpha+1,\alpha}\,(n+1)\,(\varepsilon_{\alpha+1}+\varepsilon_\alpha)\,\frac{1/\tau_{\alpha+1,\alpha}}{\omega^{*2}+1/\tau^2_{\alpha+1,\alpha}} + \xi_1^1\frac{\sigma_1}{e}, \qquad \text{(IV-25)}$$

$$\gamma_2 = -\frac{e}{m}(\alpha_2\alpha_1)^{1/2}\sum_{\alpha} f_{\alpha+1,\alpha}\,(n+1)(\varepsilon_{\alpha+1}+\varepsilon_\alpha)\,\frac{\omega^*}{\omega^{*2}+1/\tau^2_{\alpha+1,\alpha}} + \xi_1^1\frac{\sigma_2}{e}, \qquad \text{(IV-26)}$$

$$\gamma_3 = -\frac{e}{m}\left(\frac{m\alpha_3^2}{\hbar^2\alpha_{11}}\right)\sum_{\alpha}(\hbar k_z)^2 f_{\alpha\alpha}\tau_{\alpha\alpha} + \frac{\alpha_{13}}{\alpha_{11}}\xi_1^1\sigma_3, \qquad \text{(IV-27)}$$

from equation (IV-2) one finds the complete tensor $\underline{\underline{\gamma}}$:

$$\underline{\underline{\gamma}} = \begin{pmatrix} \gamma_1 & -\gamma_2 & -\frac{\alpha_{13}}{\alpha_{11}}\gamma_1 \\ \gamma_2 & \frac{\alpha_1}{\alpha_{11}}\gamma_1 & \frac{\alpha_{13}}{\alpha_{11}}\gamma_2 \\ \frac{\alpha_{13}}{\alpha_{11}}\gamma_1 & \frac{\alpha_{13}}{\alpha_{11}}\gamma_2 & \frac{\alpha_{13}}{\alpha_{11}}\gamma_1 + \gamma_3 \end{pmatrix}. \qquad \text{(IV-28)}$$

In the laboratory system, we assume that $\bar{B}$, parallel to the z-axis, is at an angle θ relative to the longitudinal ellipsoidal axis, and that $\bar{\mathcal{E}}$, parallel to the x-axis, is at angle ϕ relative to the plane containing $\bar{B}$ and the ellipsoidal axis. Taking into account the four-valley model for n-Germanium, the conductivity tensor $\underline{\underline{\sigma}}$ thus has the form:

$$\begin{pmatrix} \sum_{r=1}^{4}\sigma_1^r\left(\cos\phi_r + \frac{\alpha_1}{\alpha_{11}^r}\sin^2\phi_r\right) & \sum_{r=1}^{4}\sigma_1^r\left(1-\frac{\alpha_1}{\alpha_{11}^r}\right)\sin\phi_r\cos\phi_r - \sigma_2^r & \sum_{r=1}^{4}\frac{\alpha_{13}^r}{\alpha_{11}^r}\left(\sigma_1^r\cos\phi_r + \sigma_2^r\sin\phi_r\right) \\ \sum_{r=1}^{4}\sigma_1^r\left(1-\frac{\alpha_1}{\alpha_{11}^r}\right)\sin\phi_r\cos\phi_r + \sigma_2^r & \sum_{r=1}^{4}\sigma_1^r\left(\sin^2\phi_r + \frac{\alpha_1}{\alpha_{11}^r}\cos^2\phi_r\right) & \sum_{r=1}^{4}\frac{\alpha_{13}^r}{\alpha_{11}^r}\left(\sigma_1^r\sin\phi_r + \sigma_2^r\cos\phi_r\right) \\ \sum_{r=1}^{4}\left(\sigma_1^r\cos\phi_r - \sigma_2^r\sin\phi_r\right)\frac{\alpha_{13}^r}{\alpha_{11}^r} & \sum_{r=1}^{4}\frac{\alpha_{13}^r}{\alpha_{11}^r}\left(\sigma_1^r\sin\phi_r + \sigma_2^r\cos\phi_r\right) & \sum_{r=1}^{4}\frac{\alpha_{13}^r}{\alpha_{11}^r}\sigma_1^r + \sigma_3^r \end{pmatrix}, \qquad \text{(IV-29)}$$

where r stands for a valley, ranging from 1 to 4, and

$$\sigma_1^r = \frac{e^2}{m}\alpha_{11}^r \sum_{\alpha} f_{\alpha+1,\alpha}^r (n+1) \frac{1/\tau_{\alpha+1,\alpha}^r}{(\omega^{*r})^2 + 1/(\tau_{\alpha+1,\alpha}^r)^2} , \tag{IV-30}$$

$$\sigma_2^r = \frac{e^2}{m}(\alpha_{11}^r)^{1/2} \sum_{\alpha} f_{\alpha+1,\alpha}(n+1) \frac{\omega^{*r}}{(\omega^{*r})^2 + 1/(\tau_{\alpha+1,\alpha}^r)^2} , \tag{IV-31}$$

$$\sigma_3^r = \frac{e^2}{m}\left(\frac{m\alpha_3^2}{\hbar^2\alpha_1^r}\right) \sum (\hbar k_z)^2 f_{\alpha\alpha}^r \tau_{\alpha\alpha}^r , \tag{IV-32}$$

$$\alpha_{11}^r = \alpha_1 \cos^2\theta_r + \alpha_3 \sin\theta_r , \tag{IV-33}$$

$$\omega^{*r} = (\alpha_1 \alpha_{11}^r)^{1/2} \omega , \tag{IV-34}$$

$$m^{*r} = \frac{\alpha_{11}^r}{\alpha_1 \alpha_3} m , \tag{IV-35}$$

$$\frac{1}{\tau_{\alpha+1,\alpha}^r} = \frac{A}{(2\pi\lambda)^2}\left(\frac{2m^{*r}}{\hbar^2}\right)^{1/2} \sum_{\alpha_y \pm}{}' \left[\varepsilon - (n+\tfrac{1}{2})\hbar\omega^{*r} \pm \gamma_p \hbar \frac{v_e}{\lambda}\right]^{-1/2} , \tag{IV-36}$$

$$f_{\alpha}^r = e^{-(\varepsilon_{\alpha}^r - \xi_1)/kT} , \tag{IV-37}$$

$$\varepsilon_{\alpha}^r = (n+1/2)\hbar\omega^{*r} + \frac{\hbar^2 k_z^2}{2m^{*r}} , \tag{IV-38}$$

The $\underline{\underline{\gamma}}$-tensor should have a transformation similar to that given by equation (IV-29):

$$\begin{pmatrix} \sum_{r=1}^{4} \gamma_1^r \left(\cos^2\phi_r + \frac{\alpha_1}{\alpha_{11}^r}\sin^2\phi_r\right) & \sum_{r=1}^{4} \gamma_1^r \left(1 - \frac{\alpha_1}{\alpha_{11}^r}\right)\sin\phi_r\cos\phi_r - \gamma_2^r & \sum_{r=1}^{4} \frac{\alpha_{13}^r}{\alpha_{11}^r}\left(\gamma_1^r\cos\phi_r + \gamma_2^r\sin\phi_r\right) \\ \sum_{r=1}^{4} \alpha_1^r \left(1 - \frac{\alpha_1}{\alpha_{11}^r}\right)\sin\phi_r\cos\phi_r - \gamma_2^r & \sum_{r=1}^{4} \gamma_1^r \left(\sin^2\phi_r + \frac{\alpha_1}{\alpha_{11}^r}\cos^2\phi_r\right) & \sum_{r=1}^{4} \frac{\alpha_{13}^r}{\alpha_{11}^r}\left(\gamma_1^r\sin\phi_r + \gamma_2^r\cos\phi_r\right) \\ \sum_{r=1}^{4} \frac{\alpha_{13}^r}{\alpha_{11}^r}\left(\gamma_1^r\cos\phi_r - \gamma_2^r\sin\phi_r\right) & \sum_{r=1}^{4} \frac{\alpha_{13}^r}{\alpha_{11}^r}\left(\gamma_1^r\sin\phi_r + \gamma_2^r\cos\phi_r\right) & \sum_{r=1}^{4} \frac{\alpha_{13}^r}{\alpha_{11}^r}\gamma_1^r + \gamma_2^r \end{pmatrix} \tag{IV-39}$$

with

$$\gamma_1^r = -\frac{e}{m}\alpha_{11}^r \sum_{\alpha} f_{\alpha+1,\alpha}^r (n+1)(\varepsilon_{\alpha+1}^r + \varepsilon_{\alpha}^r) \frac{\omega^{*r}}{\omega^{*r2} + \tau_{\alpha,\alpha+1}^{-2}} \tag{IV-40}$$

$$\nu_2 = -\frac{e}{m}\left(\alpha_n^r \alpha_l\right)^{n_2} \sum f^r_{\alpha n+1,\alpha}\,(n+1)\left(\varepsilon^r_{\alpha n+1} + \varepsilon^r_{\alpha}\right) \frac{\omega^{*r}}{(\omega^{*r})^2 + 1/(\tau^r_{\alpha n+1,\alpha})^2} + q^r \frac{\alpha_2}{e}, \tag{IV-41}$$

$$\nu_3 = -\frac{e}{m}\left(\frac{m\alpha_3^2}{k^2 \alpha_n}\right) \sum_{\alpha} (k\,k_2)^2 f^r_{\alpha\alpha}\,\tau^r_{\alpha\alpha} + \frac{\alpha_3^r}{\alpha_n^r}\frac{q^r}{e}\sigma_3 \quad . \tag{IV-42}$$

CHAPTER V

APPLICATION TO n-Ge AND CONCLUSION

In the following calculations, we check the validity of our formalism by making comparison with the existing experimental data.

Germanium is an indirect band gap semiconductor with diamond structure, which consists of two identical interlocking face-centered cubic lattices. There is a set of eight equivalent minimum energy points which lie along the $\langle 111 \rangle$ directions in $\bar{k}$-space at the intersection of those directions with the surface of the Brillouin zone.

These minima thus lie at the center of the hexagonal face of the Brillouin zone. The constant-energy surfaces are again ellipsoidal in form, but the energy minima are at the zone boundary, and since there is a rather large forbidden energy region which must be surmounted before the electron can be excited outside the Brillouin zone in these directions, there are eight half-ellipsoids in the interior of the Brillouin zone along the $\langle 111 \rangle$ directions. For many purposes these may be considered to be equivalent to four full ellipsoids.

In calculating the transport properties of a crystal in which the energy surface has the form

$$E(k) = \frac{\hbar^2}{2m}\left[\alpha_1(k_x - k_{x_0})^2 + \alpha_2(k_y - k_{y_0})^2 + \alpha_3(k_z - k_{z_0})^2\right], \qquad \text{(V-1)}$$

one can calculate the effect due to one ellipsoid and sum over all ellipsoids.

We will consider, for convenience, four valleys lying along $\langle 111 \rangle$ (valley 1), $\langle \bar{1}11 \rangle$ (valley 2), $\langle \bar{1}\bar{1}1 \rangle$ (valley 3) and $\langle 1\bar{1}1 \rangle$ (valley 4) when the applied magnetic field is in the [001] direction and the electric

field is in the [100] direction.

We then have

$$\theta_1 = \theta_2 = \theta_3 = \theta_4 = 54.7^\circ \tag{V-2}$$

and $\phi_1 = 45^\circ$, $\phi_2 = 135^\circ$, $\phi_3 = -135^\circ$, $\phi_4 = -45^\circ$

Putting these values for θ in the equations (IV-29, IV-39), the components $\sigma_{13}, \sigma_{23}, \sigma_{31}, \sigma_{32}, \gamma_{13}, \gamma_{23}, \gamma_{31}, \gamma_{32}$ will be equal to zero. The conductivity tensor takes the form

$$\underline{\underline{\sigma}} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & 0 \\ \sigma_{21} & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{pmatrix} \tag{V-3}$$

where $$\sigma_{11} = \sum_r \sigma_1^r \left(\cos^2\phi_r + \frac{\alpha_1}{\alpha_{11}^r} \sin^2\phi_r \right), \tag{V-4}$$

$$\sigma_{12} = -\sum_r \sigma_2^r \quad , \tag{V-5}$$

$$\sigma_{21} = \sum_r \sigma_2^r \quad , \tag{V-6}$$

$$\sigma_{22} = \sum_r \sigma_1^r \left(\sin^2\phi_r + \frac{\alpha_1}{\alpha_{11}^r} \cos^2\phi_r \right), \tag{V-7}$$

$$\sigma_{33} = \sum_r \left(\frac{\alpha_{13}^r}{\alpha_{11}^r} \sigma_1^r + \sigma_3^r \right), \tag{V-8}$$

and the $\underline{\underline{\nu}}$ tensor takes the form

$$\underline{\underline{\nu}} = \begin{pmatrix} \nu_{11} & \nu_{12} & 0 \\ \nu_{21} & \nu_{22} & 0 \\ 0 & 0 & \nu_{33} \end{pmatrix}$$

where $$\nu_{11} = \sum_r \nu_1^r \left(\cos^2\phi_r + \frac{\alpha_1}{\alpha_{11}^r} \sin^2\phi_r \right) \tag{V-10}$$

$$\nu_{12} = -\sum_r \nu_2^r \tag{V-11}$$

$$\nu_{21} = \sum_r \nu_2^r \tag{V-12}$$

$$\gamma_{22} = \sum_r \gamma_i^r (\sin^2\phi_r + \frac{\alpha_1}{\alpha_i^r}\cos^2\phi_r) \,, \tag{V-13}$$

$$\gamma_{33} = \sum_r \left(\frac{\alpha_{13}^r}{\alpha_{11}^r}\sigma_1^r + \sigma_3^r\right) \tag{V-14}$$

In this case $\underline{\underline{\rho}} = \underline{\underline{\sigma}}^{-1}$ can be easily found:

$$\underline{\underline{\rho}} = \begin{pmatrix} \frac{\sigma_{22}}{(\sigma_{11}\sigma_{22}+\sigma_{12}^2)} & -\frac{\sigma_{12}}{(\sigma_{11}\sigma_{22}+\sigma_{12}^2)} & 0 \\ \frac{\sigma_{21}}{(\sigma_{11}\sigma_{22}+\sigma_{21}^2)} & \frac{\sigma_{11}}{(\sigma_{11}\sigma_{22}+\sigma_{21}^2)} & 0 \\ 0 & 0 & 1/\sigma_{33} \end{pmatrix}, \tag{V-15}$$

and with the help of equation (IV-11) we are able to find the tensor :

$$\underline{\underline{Q}} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} \tag{V-16}$$

where

$$Q_{11} = (\sigma_{22}\gamma_{11} + \sigma_{12}\gamma_{22})/\tau(\sigma_{11}\sigma_{22} + \sigma_{12}^2) \,, \tag{V-17}$$

$$Q_{21} = -Q_{12} = (\sigma_{21}\gamma_{11} + \sigma_{11}\gamma_{12})/\tau(\sigma_{11}\sigma_{22} + \sigma_{21}^2) \,, \tag{V-18}$$

$$Q_{22} = (\sigma_{11}\gamma_{22} - \sigma_{12}\gamma_{11})/\tau(\sigma_{11}\sigma_{22} - \sigma_{21}^2) \,, \tag{V-19}$$

$$Q_{33} = \frac{1}{\tau}\frac{\gamma_{33}}{\sigma_{33}} \,, \tag{V-20}$$

$$Q_{13} = Q_{23} = Q_{31} = Q_{32} = 0 \tag{V-21}$$

In order to have the conductivity tensor and $\underline{\underline{\alpha}}$ -tensor in a suitable form for computer calculation, we divide the $\bar{k}$ -space into cells such that

$$\frac{\hbar^2 k_z^2}{2m^*} = (n'' + x^4)\,\hbar\,\omega_j^* \tag{V-22}$$

where n'' is an integer and x , a fraction lying between 0 and 1. x^4 is chosen instead of x for convenience in integration by Simpson's rule.

We will change the summation over k to an integration such that:

$$\sum \rightarrow \frac{1}{(2\pi\lambda)^2}\int dk_y = \frac{4}{(2\pi\lambda)^2}\int_0^1 \frac{x^3 dx}{(n''+x^4)^{1/2}}\left(\frac{2m^*\omega^*}{\hbar}\right)^{1/2}. \qquad \text{(V-23)}$$

Here we have assumed that the crystal has a unit volume and that the center of the cyclotron orbit lies on the x-axis at some point x_k between -1/2 and 1/2. Since $x_k = x^2 k_y$, then we have

$$-\frac{1}{2\lambda^2} \leq k_y \leq \frac{1}{2\lambda^2}, \qquad \text{(V-24)}$$

and using the equation (V-22) $\mathcal{E}_\alpha$ and f_α can be written as

$$\mathcal{E}_\alpha = (N + x^4 + \tfrac{1}{2})\hbar\omega^* \qquad \text{(V-25)}$$

$$f_\alpha = e^{\mathcal{E}_F/kT} e^{-(N+x^2+\frac{1}{2})\alpha}, \qquad \text{(V-26)}$$

where $$N = n + n'', \qquad \text{(V-27)}$$

and $$\alpha = \frac{\hbar\omega^*}{kT} \qquad \text{(V-28)}$$

Also we have:

$$\frac{1}{\tau_\alpha} \rightarrow \frac{1}{\tau_{n_x}} = A_1 \sum' \left\{\left[(N'+x^4)\hbar\omega^* + \nu_p \frac{\hbar u_g}{\lambda}\right]^{-1/2} + \left[(N'+x^4)\hbar\omega^* - \nu_p \frac{\hbar u_g}{\lambda}\right]\right\} \qquad \text{(V-29)}$$

with $$A_1 = \frac{2\pi kT E_1^2}{\hbar \rho_e u_g^2}\left(\frac{2m^*}{\hbar^2}\right)^{1/2}\frac{1}{(2\pi\lambda)^2} \qquad \text{(V-30)}$$

and $$N' = n - n'$$

Putting this information in equations (IV-30, 31 and 32), we get

$$\sigma_1^r = C_1^r \int_0^1 x^4 dx\, e^{-x^4 a^r} \sum_{N=n}^{\infty} e^{-(N+\frac{1}{2})a^r}\left[N+1+x^2\sum\frac{N-n''+1}{(n''+x^4)^{1/2}}\right]\cdot\frac{2\mu^r(x)/\mu^r}{x^4+(\mu^r(x))^2} \qquad \text{(V-32)}$$

$$\sigma_2^r = C_2^r \int_0^1 x^4 dx\, e^{-x^4 a^r} \sum_{N=n}^{\infty} e^{-(N+\frac{1}{2})a^r}\left[N+1+x^2\sum\frac{N-n''+1}{(n''+x^4)^{1/2}}\right]\cdot\frac{1}{x^4+(\mu^r(x))^2} \qquad \text{(V-33)}$$

$$\sigma_3^r = C_3^r \int_0^1 x^4 dx\, e^{-x^4 a^r} \sum_{N=n}^{\infty} e^{-(N+\frac{1}{2})a^r}\left[x^2+\sum(n''+x^4)^{1/2}\right]\left[1+\frac{x}{\sum(N'+x^2)^{1/2}}\right]^{-1} \qquad \text{(V-34)}$$

where $\mu_0 = A_1/\omega^2$,

$$\mu(x) = \sum_{N'=0}^{N_0}\left\{\left[N'+x^4+\frac{\nu_p \hbar u_z}{\lambda}\right]^{-1/2}+\left[N'+x^4-\frac{\nu_p \hbar u_z}{\lambda}\right]^{-1/2}\right. \tag{V-35}$$

$$\left. + \sum\left\{\left[N'+1+x^4+\frac{\nu_p \hbar u_z}{\lambda}\right]^{-1/2}+\left[N'+1+x^4-\frac{\nu_p \hbar u_z}{\lambda}\right]^{-1/2}\right\}\right. \tag{V-36}$$

$$c_1 = \frac{e^2 \omega_{c1}}{m\omega^2} e^{\varepsilon/kT}(1-e^{-\alpha})\frac{1}{(2\pi\lambda)^2}\left(\frac{2m^*\omega^2}{\hbar}\right)^{1/2} A_1 , \tag{V-37}$$

$$c_2 = \frac{e^2}{m\omega^2}(\nu_1\nu_2)^{1/2} e^{\varepsilon/kT}(1-e^{-\alpha})\frac{1}{(2\pi\lambda)^2}\left(\frac{2m^*\omega^2}{\hbar}\right)^{1/2} \tag{V-38}$$

$$c_3 = \frac{e^2}{mA_1}\frac{a}{(2\pi\lambda)^2}\left(\frac{2m^*\omega^2}{\hbar}\right)^{1/2} . \tag{V-39}$$

An expression for $\underline{\underline{\nu}}$ can be put into integrable form in a similar way.

Equations (V-32, 33, 34) can be readily evaluated on the computer. Calculations are done for all four ellipsoids and finally a sum is taken to find the complete conductivity tensor in the laboratory frame. Usually what is measured in the laboratory is the relative change in transverse magnetoresistance $\frac{\Delta\rho_{xx}}{\rho(0)}$, the relative change in longitudinal magnetoresistance $\Delta\rho_{33}/\rho(0)$, and the reduced Hall coefficient $\bar{r}_H = -R_H n_e e c$. They can be written as:

$$\Delta\rho_{xx}/\rho(0) \equiv \frac{\sigma(0)\sigma_{22}}{(\sigma_{11}\sigma_{22}+\sigma_{21})^2} , \tag{V-40}$$

$$\Delta\rho_{33}/\rho(0) \equiv \frac{\sigma(0)}{\sigma_{33}} - 1 , \tag{V-41}$$

$$r_H \equiv -R_H n_e e c \tag{V-42}$$

where $\sigma(0)$ is the zero-field resistivity given by

$$\sigma(0) = (16e^2\hbar\rho_c u_z^2/18\pi\varepsilon_1^2 m)(\nu_1^2\nu_3)^{1/2}(2\nu_1+\nu_3)n_e(2mkT/\pi\hbar^2)^{-3/2}.$$

The relative change in transverse magnetothermal emf, $\Delta Q_{xx}/Q(0)$,

the relative change in longitudinal magnetothermal emf, $\Delta Q_{zz}/Q(0)$, and the Ettinghausen-Nerst coefficient Q_H, can be written in terms of the components of $\underline{\nu}$ and $\underline{\sigma}$:

$$\frac{\Delta Q_{xx}}{Q(0)} = \left[\frac{\nu_{11}\sigma_{22} + \nu_{12}\sigma_{21}}{T(\sigma_{11}\sigma_{22} + \sigma_{21}^2)} - 1\right], \tag{V-43}$$

$$\frac{\Delta Q_{zz}}{Q(0)} = \left[\frac{\nu_{33}}{T\sigma_{33}} - 1\right], \tag{V-44}$$

$$Q_H = \frac{\nu_{21}\sigma_{22} - \nu_{22}\sigma_{21}}{TB(\sigma_{11}\sigma_{22} + \sigma_{21}^2)}, \tag{V-45}$$

where the zero field thermoelectric power $Q(0)$ is given by:

$$Q(0) = \frac{K}{e}\left[\frac{\xi(0)}{KT} - 2\right]$$

$$e^{\xi(0)/KT} = (2mKT/\pi\hbar^2)^{-3/2}(\alpha_1^2\alpha_3)^{1/2}\eta_c .$$

In the numerical calculation, the value of α_1 and α_2 were taken to be $\alpha_1 = 12.3$, $\alpha_3 = .63$, $E_1 = 9.07$ eV. The crystal density for n-Ge is 5.32 gm/cm^3 and the average longitudinal sound velocity is 5.4×10^5 cm/sec.

Numerical values of the relative change in transverse and longitudinal magnetoresistance for a magnetic field applied in the <001> - direction at temperature T = 30°K are presented in Figure 1. The results of the transverse magnetoresistance computations agree, within the range of the approximations made, with the results of Gallagher and Love.[7] The results for the longitudinal magnetoresistance agree with those of Love and Wei.[21] This probably indicates the fact that our assumption of predominant acoustic-phonon scattering is valid.

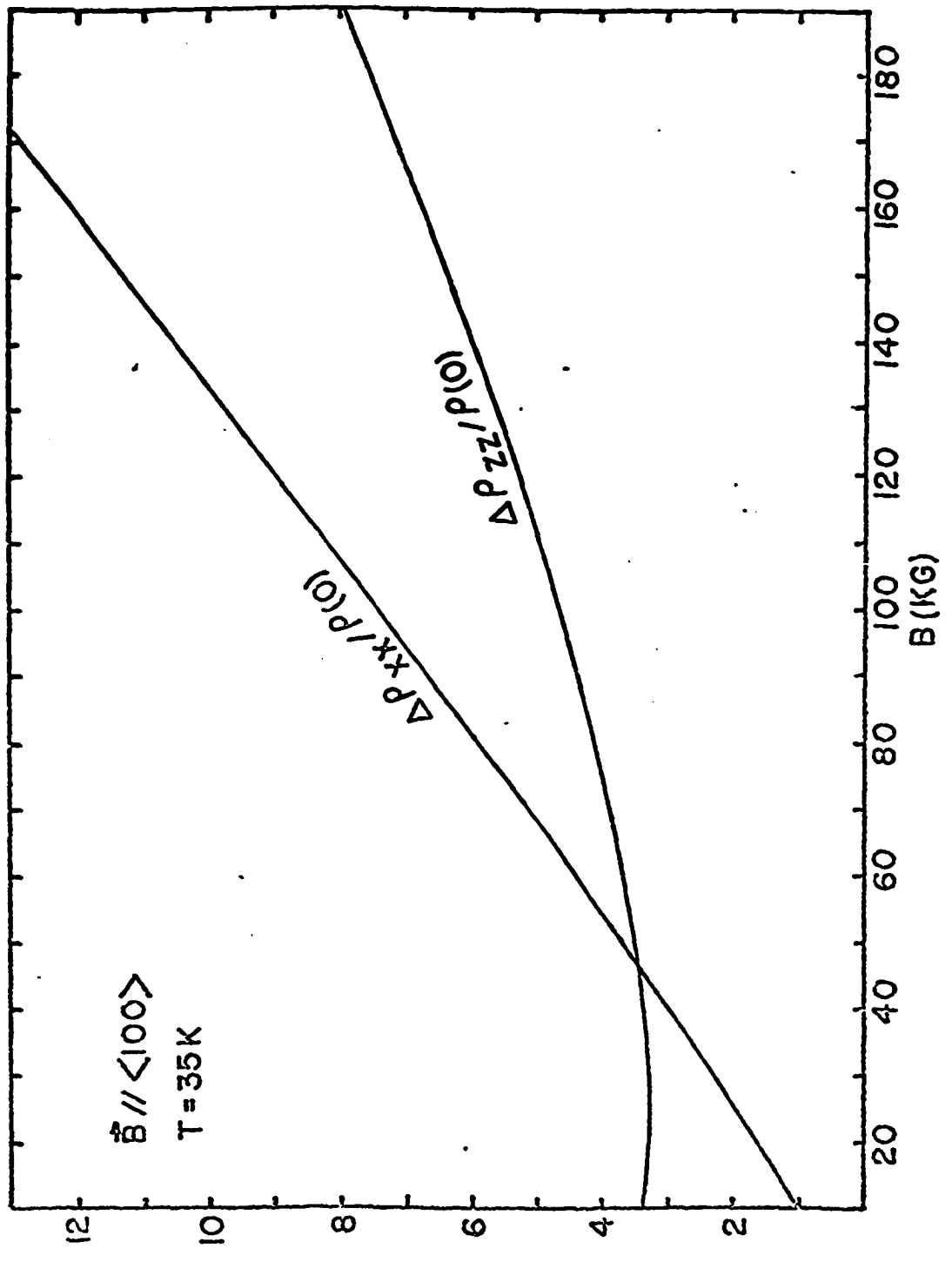
In Figure 2 we show the relative change in transverse and longitudinal magnetothermal emf. The functional forms of these curves are similar to the experimental curves of Puri and Geballe.[6] The values are an order of magnitude smaller than those observed experimentally. The cause of this disagreement is likely due to the fact that we do not consider here the phonon-drag contribution to the magnetothermal emf. The importance of the drag effect was first pointed out by L. E. Gurevich;[22] this effect continues to be the object of both theoretical and experimental research.

The heat current consists of three parts: a part determined by the motions of electrons, a part determined by those phonons which interact with the carriers, and finally, a part determined by the motion of the remaining phonons.

Thus it is possible to define the following three relaxation times: τ', the relaxation time of the carriers with scattering only by longitudinal acoustic phonons; τ_p, the relaxation time for the long-wave length phonons; and τ_{pe}, the relaxation time of those phonons during scattering by current carriers only. In this thesis, we consider only the first contribution (electrons-acoustic phonons scattering) to the heat current, which should be the main contribution. In order to take into account the other contributions implied by the Arora-Miller theory, we only have to find the density matrix for the coupled electron-phonon system. The interesting subject of the phonon-drag contribution is left for further studies.

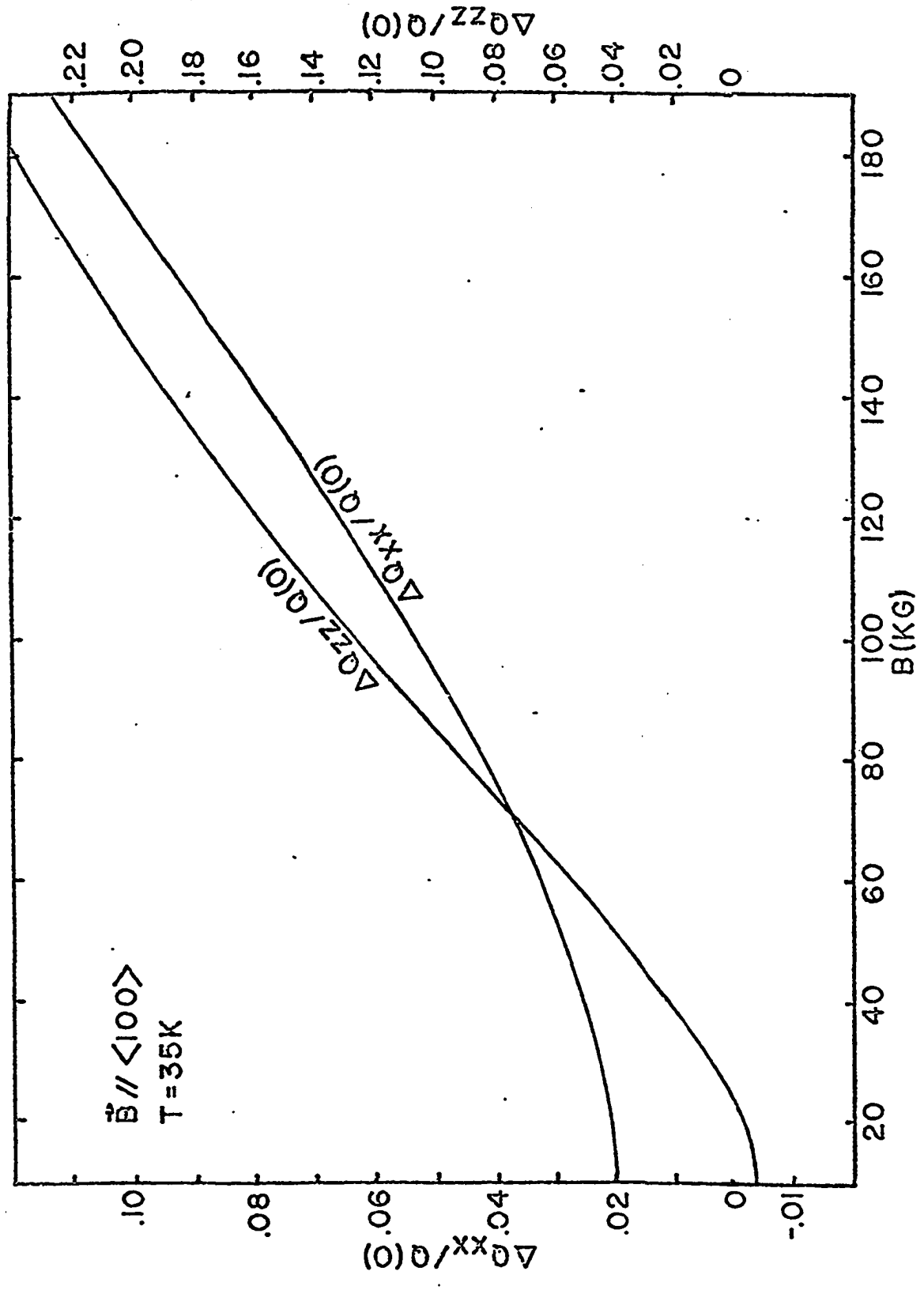
APPENDIX A

Fig. 1. Ohmic magnetoresistance as a function of magnetic field B for $\vec{B} \parallel \langle 100 \rangle$ and T = 35K for parameters appropriate to n-Germanium



APPENDIX B

Fig. 2. Electronic contribution to the magnetothermal emf as a function of magnetic field B for $\vec{B} \parallel \langle 100 \rangle$ and T = 35K for parameters appropriate to n-Germanium.



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