

Evaluation of Transport Integrals for Mixed Scattering and Application to Galvanomagnetic Effect*

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The Johnson-Whitesell evaluations of the conductivity integrals for mixed scattering have been extended over larger ranges of magnetic field and impurity scattering parameters to allow their application to the high-mobility semiconductors. Values are given for the first thermoelectric integral. Use of the magnetic field dependence of galvanomagnetic and thermomagnetic properties to study charge-carrier scattering is discussed. Applications of the functions in the analysis of Hall effect, Corbino magnetoresistance, and thermomagnetic phenomena as functions of magnetic field are illustrated.

I. INTRODUCTION

AN approximate determination of the extent of impurity scattering present in a semiconductor has usually been accomplished by comparing the mobility measured on the specimen with values which have been determined on other specimens as a function of impurity concentration and extrapolated to the limit of zero impurity concentration.¹ When applied to new semiconductors this procedure involves extensive experimental data and is, of course, subject to uncertainties arising from the fact that specimens produced with different impurity contents may also differ in other significant aspects. For example, there can be variations in crystal perfection, degree of impurity compensation, and so forth. For obtaining information on charge carrier scattering, there are therefore distinct advantages in devising measurements and analyses which can be carried out on a single specimen. Certain possibilities are galvanomagnetic and thermomagnetic phenomena. In the weak magnetic field region, the conductivity involves averages of the first power of the relaxation time; the Hall effect involves the square of the relaxation time, and the magnetoresistance involves the cube of the relaxation time.² In the strong-field region, however, the cross-effect coefficients become independent of the relaxation time.³ Hence, it follows that measurements of electrical properties as functions of magnetic field can yield helpful information.⁴

In the past, it has been difficult to realize the strong-field region with ordinary laboratory magnetic fields.

In the case of the high-mobility semiconductors, which are now being studied, this problem no longer exists since it is actually the dimensionless parameter μH which enters into the equations for the galvanomagnetic effects. However, the analysis of the results when both lattice and impurity scattering occur is impeded by the fact that the transport integrals cannot be evaluated analytically. Numerical evaluations were initially carried out by Johnson and Whitesell,⁵ but the tabulation is not sufficiently extensive to encompass the region from weak to strong magnetic fields nor to include sufficient degrees of impurity scattering. It is for this reason that the Johnson-Whitesell calculations were extended.

II. DISCUSSION OF THE FUNCTIONS

The principal functions are defined as follows:

$$K(\beta, \gamma) \equiv \int_0^{\infty} \frac{x^3 e^{-x} (x^2 + \beta) dx}{(x^2 + \beta)^2 + \gamma x^3}, \quad (1)$$

$$L(\beta, \gamma) \equiv \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{x^{3/2} e^{-x} dx}{(x^2 + \beta)^2 + \gamma x^3}. \quad (2)$$

The magnetic field parameter γ is defined by

$$\gamma \equiv \frac{9}{16} \pi (\mu_L^0 H)^2, \quad (3)$$

and the impurity scattering parameter β has been approximated^{4,5} by

$$\beta = 6\mu_L^0 / \mu_I^0. \quad (4)$$

A discussion concerning this approximation is given in Sec. IV.

For $\beta=0$, the integrals K and L can be evaluated analytically in terms of exponential integrals and error functions, while for $\gamma=0$, the solutions involve sine and cosine integrals and the Fresnel integrals. Power series

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¹ See, for example: E. M. Conwell, *Proc. Inst. Radio Engrs.* **40**, 1327 (1952); M. B. Prince, *Phys. Rev.* **92**, 681 (1953).

² See, for example: Harvey Brooks, *Advances in Electronics and Electron Physics* (Academic Press, Inc., New York, 1955), Vol. 7, p. 128.

³ In the case of quadratic energy surfaces this is apparent from the way in which the relaxation time is present in the integrands, namely, $\tau^2(1+\omega_0^2\tau^2)^{-1}$, where $\omega_0 = eH/m^*c$.

⁴ An example is the analysis of multiband contributions to transport phenomena. See Willardson, Harman, and Beer, *Phys. Rev.* **96**, 1512 (1954).

⁵ V. A. Johnson and W. J. Whitesell, *Phys. Rev.* **89**, 941 (1953). The notation is such that J_1 and J_2 are identical, respectively, with our K and $\frac{1}{2}\pi^3 L$. Caution must be used to avoid the typographical errors, some of which are apparent in comparing Tables I and II with IV.

TABLE III. Numerical evaluations of the thermoelectric power function, $K^{(2)}(\beta, \gamma) = \int_0^\infty \frac{x^4 e^{-x}(x^2 + \beta) dx}{(x^2 + \beta)^2 + \gamma x^3}$.

| γ/β | 0.01 | N^a | 0.1 | N | 1 | N | 10 | N |
|----------------|---------|-------|---------|-----|---------|-----|---------|-----|
| 0.1 | 1.90230 | 0 | 1.85634 | 0 | 1.58168 | 0 | 0.83600 | 0 |
| 1 | 1.40340 | 0 | 1.39770 | 0 | 1.29836 | 0 | 0.78202 | 0 |
| 10 | 0.43726 | 0 | 0.44235 | 0 | 0.47718 | 0 | 0.48568 | 0 |
| 100 | 0.57808 | 1 | 0.58651 | 1 | 0.66584 | 1 | 0.11392 | 0 |
| 1000 | 0.59861 | 2 | 0.60755 | 2 | 0.69581 | 2 | 0.14591 | 1 |

^a Each entry should be divided by that power of 10 indicated by column N .

solutions, either in β or in γ , are not possible since $\beta=0$ and $\gamma=0$ are singular points and the derivatives do not exist at these points. A single exception is the first derivative with respect to γ , which does exist at $\gamma=0$. One can therefore write

$$K(\beta, \gamma) \cong K(\beta, 0) + \left(\frac{\partial K}{\partial \gamma} \right)_{\gamma=0} \gamma, \quad \gamma \ll 1 \tag{5}$$

$$L(\beta, \gamma) \cong L(\beta, 0) + \left(\frac{\partial L}{\partial \gamma} \right)_{\gamma=0} \gamma, \quad \gamma \ll 1.$$

One differentiation under the integral sign is valid, and the results with $\gamma=0$ can again be evaluated analytically in terms of sine and cosine integrals and the Fresnel integrals. However, since the equations designated (5) are valid to approximately five significant figures for $\gamma=0.001$ and 0.003 , these derivatives, as well as the functions $K(\beta, 0)$ and $L(\beta, 0)$, can be obtained with adequate accuracy through use of those two entries in the tables. In this way, the tables can be extended to include any value of γ between 0 and 0.003.

Table I gives numerical evaluations of function (1) for values of β from 0.0001 to 300 000 and values of γ from 0.001 to 300 000 in multiples of approximately 3. A similar evaluation of function (2) is given in Table II.

The thermoelectric function is defined by

$$K^{(2)}(\beta, \gamma) \equiv \int_0^\infty \frac{x^4 e^{-x}(x^2 + \beta) dx}{(x^2 + \beta)^2 + \gamma x^3}. \tag{6}$$

Only a limited number of evaluations of $K^{(2)}$ were done. In many cases, however, the ratio $K^{(2)}/K$ is a much more slowly varying function than is $K^{(2)}$. Therefore, a fairly accurate interpolation to include values of γ or β for which the $K(\beta, \gamma)$ are tabulated is possible.

Table III gives numerical evaluations of function (6) for values of β from 0.01 to 10 and γ from 0.1 to 1000 in multiples of 10.

III. APPLICATION OF THE FUNCTIONS

A. Hall Effect

Use of the tabulations to analyze Hall effect and magnetoresistance in a semiconductor of simple band structure has already been discussed by Johnson and Whitesell.⁵ In the case of degenerate bands where two bands contribute to the extrinsic conduction processes, results are much more striking. To illustrate, the Hall coefficient factor, R_H/R_∞ is shown in Figs. 1 and 2 for various degrees of impurity scattering and two ratios of fast hole densities and mobilities. For these calculations, the extrinsic Hall effect equations have been modified to include the contribution of the fast hole band⁴ to yield

$$\frac{R_H}{R_\infty} = \frac{3\pi}{8} \left(1 + \frac{n_3}{n_2} \right) \left\{ \frac{L(\beta_2, \gamma_2) + \left(\frac{\sigma_{L,3}^0}{\sigma_{L,2}^0} \right) \left(\frac{\mu_{L,3}^0}{\mu_{L,2}^0} \right) L(\beta_3, \gamma_3)}{\left[K(\beta_2, \gamma_2) + \left(\frac{\sigma_{L,3}^0}{\sigma_{L,2}^0} \right) K(\beta_3, \gamma_3) \right]^2 + \frac{1}{4} \pi \gamma_2 \left[L(\beta_2, \gamma_2) + \left(\frac{\sigma_{L,3}^0}{\sigma_{L,2}^0} \right) \left(\frac{\mu_{L,3}^0}{\mu_{L,2}^0} \right) L(\beta_3, \gamma_3) \right]^2} \right\}. \tag{7}$$

In all cases, the mobility of the slow holes is taken as 45 000 cm²/volt-sec.⁶

In Fig. 1, the density ratio of fast and slow holes is 0.018, with a mobility ratio of 10; in Fig. 2 the values are, respectively, 0.1 and $\sqrt{10}$. The effects are most striking when the mobility ratio is large, as is true for Fig. 1. Here, it is seen that the weak-field Hall coefficient is especially sensitive to β , the impurity scattering parameter defined in Eq. (4). A small amount of impurity scattering lowers the Hall curve significantly at weak fields and slightly at intermediate field strengths.

⁶ Although the mobility value is indicative of germanium at 77°K, the examples are intended only to be illustrative and the magnitudes of the other parameters may not necessarily apply. The notation is that used in reference 4 with subscripts 2 and 3 referring to the slow and fast holes, respectively.

Additional impurity scattering further lowers the curve at weak fields but raises it at intermediate field strengths. This is caused by the fact that the saturation effects are delayed. Further increases in β raise the Hall curves in both regions and delay saturation until higher field strengths are reached. An interesting observation concerns that value of β for which the Hall coefficient factor is a minimum. In the case of a single band it was found to occur at $\beta=0.67$.⁵ For two-band conduction with the characteristics of each band as stated above, the minimum is seen to occur for values of β in the neighborhood of 3.

A practical consequence of the calculations illustrated by Fig. 1 is the suggestion that in order to approximate closely the weak-field plateau, Hall measurements must

be taken at magnetic field strengths below 50 gauss. For impurity scattering corresponding to $\beta > 1$, this value may be increased to 100 gauss.

The effect of decreasing the fast-hole mobility is to increase greatly the weak-field plateau, even at rather small amounts of impurity scattering, as indicated in Fig. 2.

B. Magnetoresistance Effects

The effect of impurity scattering on the ordinary transverse magnetoresistance coefficient, $\Delta\rho/\rho H^2$, is very great in the weak magnetic field region. Results are presented by Appel⁷ for a single band and for a two-band model with electrons and holes in the case of the pure lattice scattering. Recently, Becker⁸ has completed calculations for the case of mixed scattering when two types of holes are present, showing that only a small amount of ionized impurity scattering of the fast holes can appreciably reduce the magnetoresistance coefficient at weak magnetic fields. He also illustrates

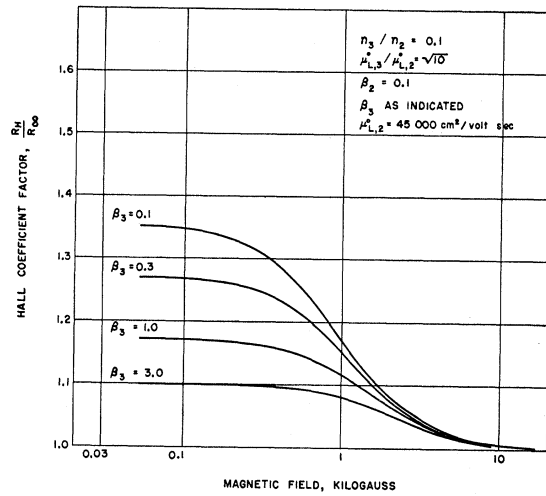


FIG. 2. Effect of impurity scattering on extrinsic Hall coefficient factor for the case of a small ratio of moderately fast holes.

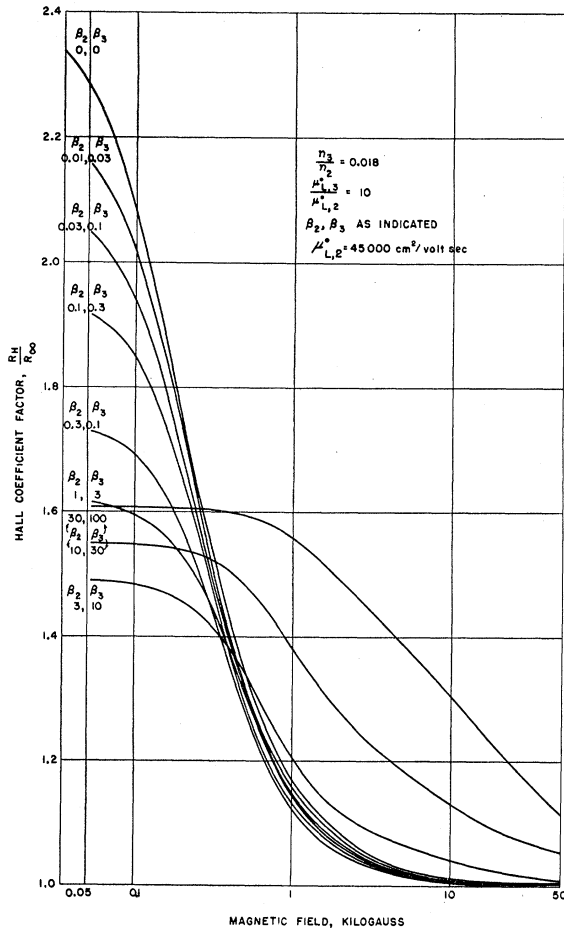


FIG. 1. Effect of impurity scattering on extrinsic Hall coefficient factor for the case of a small ratio of fairly fast holes.

⁷ J. Appel, Z. Naturforsch. **9a**, 167 (1954).

⁸ J. H. Becker, Bull. Am. Phys. Soc. Ser. II, **2**, 57 (1957).

A detailed article will appear as a National Bureau of Standards Report.

how the approximation of the relaxation time by a simple power dependence on energy produces large discrepancies when one attempts to account for magnitudes of both the Hall and the magnetoresistance effects in cases when mixed lattice-ion scattering occurs.

Therefore, we shall limit our illustrations to the Corbino magnetoresistance.⁹ Because of the boundary condition that the transverse electric field be zero, the cross-effect terms (namely, the L coefficients in the present notation) drop out of the transport equations. One can therefore obtain directly the conductivity mobility rather than the Hall mobility from galvanomagnetic measurements. At weak fields, the Corbino magnetoresistance is relatively insensitive to impurity scattering. Also, the contributions of the charge carriers do not depend on their sign. Therefore, the Corbino effect is especially suitable for analyzing semiconductors in the intrinsic region, especially when electrons and holes have significantly different mobilities. Although measurements are usually carried out with a Corbino disk having metal contacts plated along the periphery and at the center of the disk, similar results are achieved in rectangular specimens of large width-length ratios.¹⁰

In terms of the function $K(\beta, \gamma)$, the Corbino effect is given as follows¹¹:

$$\left(\frac{\Delta\rho}{\rho_0}\right)_{E_y=0} = \frac{\sigma_{L,1}^0 K(\beta_1, 0) + \sigma_{L,2}^0 K(\beta_2, 0)}{\sigma_{L,1}^0 K(\beta_1, \gamma_1) + \sigma_{L,2}^0 K(\beta_2, \gamma_2)} - 1, \quad (8)$$

⁹ For discussion of the Corbino effect, see E. P. Adams, Proc. Am. Phil. Soc. **54**, 47 (1915); H. Weiss and H. Welker, Z. Physik **138**, 322 (1954).

¹⁰ O. Madelung, Naturwiss. **42**, 406 (1955). This arrangement has also been used by C. Goldberg in magnetoconductivity analyses of germanium [Bull. Am. Phys. Soc. Ser. II, **2**, 65 (1957)].

¹¹ Derivation of the equations in this section is straightforward and details are omitted. Further information, as well as the use of data to determine electron and hole mobilities in intrinsic InSb, can be found in A. C. Beer *et al.*, "Research and development work on semiconducting materials of unusually high mobility," Office of Technical Services Report PB-121288 (unpublished).

where $\sigma_{L,1}^0$ and $\sigma_{L,2}^0$ are the conductivities due to electrons and holes, respectively, in the absence of magnetic field and impurity scattering. The impurity scattering parameter and the magnetic field parameter are defined as in Eqs. (4) and (3), respectively, the mobility and magnetic fields being in consistent units. Instead of saturating at large fields, the Corbino effect due to a single carrier continues with an H^2 dependence as indicated below:

$$\left(\frac{\Delta\rho}{\rho_0}\right)_{E_y=0} \approx \frac{9\pi}{32}(\mu_L^0 H)^2, \text{ lattice scattering, } \mu_L^0 H \gg 1, \quad (9)$$

$$\left(\frac{\Delta\rho}{\rho_0}\right)_{E_y=0} \approx \frac{3\pi}{32}(\mu_I^0 H)^2, \text{ impurity scattering, } \mu_I^0 H \gg 1. \quad (10)$$

When Corbino disk measurements are taken on intrinsic InSb where $\mu_1^0 \sim 80\mu_2^0$, only the electrons make a significant contribution at weak magnetic fields, as can be seen from the following equation:

$$\left(\frac{\Delta\rho}{\rho_0}\right)_{E_y=0} \approx \frac{9\pi}{16}(\mu_1^0 H)^2 \left[\frac{1 + (\mu_2^0/\mu_1^0)^3}{1 + (\mu_2^0/\mu_1^0)} \right], \text{ weak field, } \text{lattice scattering, } \mu_1^0 H \ll 1. \quad (11)$$

However, as H is increased, the holes become more important and the curve drops away from the H^2 line. Finally, when the holes are also in the strong-field region, the following relationship applies:

$$\left(\frac{\Delta\rho}{\rho_0}\right)_{E_y=0} \approx \frac{9\pi}{32}\mu_1^0\mu_2^0 H^2, \text{ strong field, } \text{lattice scattering, } \mu_2^0 H \gg 1. \quad (12)$$

For the case of mixed scattering, several examples somewhat representative of InSb were calculated using Eq. (8), and the results are shown in Fig. 3. It is seen

$$(Q)_{E_y=0} \equiv \frac{E_x}{\partial T/\partial x} = -\frac{k}{|e|} \left(\frac{\sigma_{L,1}^0 [K^{(2)}(\beta_1, \gamma_1) - \eta_1 K(\beta_1, \gamma_1)] - \sigma_{L,2}^0 [K^{(2)}(\beta_2, \gamma_2) - \eta_2 K(\beta_2, \gamma_2)]}{\sigma_{L,1}^0 K(\beta_1, \gamma_1) + \sigma_{L,2}^0 K(\beta_2, \gamma_2)} \right), \quad (14)$$

where $K^{(2)}$ and K are the functions defined and tabulated in the foregoing sections; η is the reduced Fermi level measured from the bottom of the conduction band (positive upward) for electrons, and from the top of the valence band (positive downward) for holes, so that $\eta_1 + \eta_2 = -E_G/kT$.

The calculations performed with Eq. (14) were done for parameters representative of intrinsic InSb at room

temperature. Hence, the partial conductivities can be replaced by the mobilities and also β_2 can be taken as zero. However β_1 , although small, will not be negligible because of electron-hole scattering which, due to the large hole-electron mass ratios, can be treated as an impurity scattering. Under these conditions Eq. (14) reduces to

$$(Q)_{E_y=0} = -\frac{k}{|e|} \left(\frac{\mu_{L,1}^0 [K^{(2)}(\beta_1, \gamma_1) - \eta_1 K(\beta_1, \gamma_1)] - \mu_{L,2}^0 [2 - (\gamma_2 + \eta_2) K(0, \gamma_2)]}{\mu_{L,1}^0 K(\beta_1, \gamma_1) + \mu_{L,2}^0 K(0, \gamma_2)} \right). \quad (15)$$

¹² Preliminary accounts of these measurements on InSb were given by R. K. Willardson and A. C. Beer, *Bull. Am. Phys. Soc. Ser. II*, **1**, 54 (1956).

¹³ For a discussion of the theory of thermoelectric and thermomagnetic effects in semiconductors, consult P. J. Price, *Phys. Rev.* **104**, 1223 (1956) and literature referenced therein.

C. Thermomagnetic Measurements

Also of interest in investigating high-mobility semiconductors is a thermomagnetic effect investigated by Willardson and Beer,¹² defined under the condition that the transverse electric and thermal gradients be zero. It is therefore the thermomagnetic analog of the Corbino effect. An important advantage to measuring this quantity is that one avoids the dilemma of trying to reconcile the simpler theory derived for isothermal transverse boundary conditions with measurements which are often more realistically described by adiabatic conditions. Also, a great simplicity in analysis is afforded by the fact that, as in the Corbino effect, the cross-effect transport coefficients (the L integrals in this case) are eliminated.¹³

A convenient means of measuring this thermomagnetic effect is to contact the semiconductor in the shape of a Corbino disk between two concentric copper cylinders maintained at temperatures T_1 and T_2 and to measure the potential difference ΔV between the copper cylinders. Then

$$[Q(H)]_{E_y=0} = \lim_{\Delta T \rightarrow 0} \left(\frac{\Delta V(H)}{\Delta T} \right). \quad (13)$$

The transport equations for simple conduction and valence bands yield, for the boundary conditions $E_y = \partial T/\partial y = j_x = 0$:

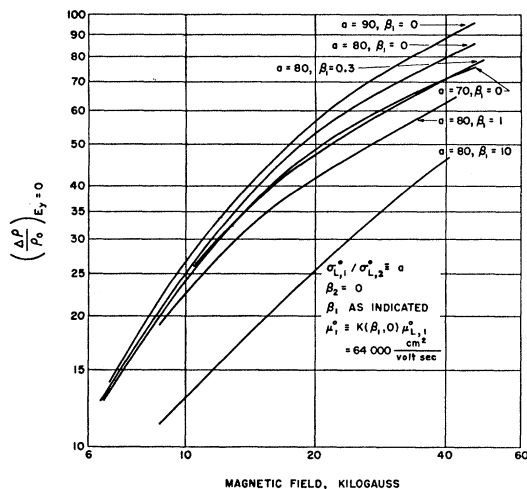


FIG. 3. Corbino magnetoresistance for various degrees of electron-ion scattering and various electron-hole conductivity ratios.

Results are shown in Fig. 4. The effect of a small amount of impurity scattering is to render the thermomagnetic effect more positive at intermediate and high-field strengths and more negative at weak fields. It is especially interesting to note the disappearance of the minimum as β increases above 0.3.

IV. COMMENTS ON APPLICATIONS OF THE FUNCTIONS IN ANALYZING DATA IN SEMICONDUCTORS

It is believed that the use of mixed scattering theory and the measurement of galvanomagnetic properties of semiconductors as a function of magnetic field can be very helpful in studying relationships between structural characteristics and transport phenomena. A limited number of illustrations were given in the preceding section. However, realization must be made of the region of applicability of the results which were presented. There are pertinent limitations imposed as a result of the derivation of the relationships.

In the first place, all equations were derived under the assumption of spherical energy surfaces. Extension to more general quadratic surfaces is readily possible, however, as has been done by Abelès and Meiboom,¹⁴ and by Shibuya.¹⁵

More serious is the fact that in the evaluation of the transport integrals, the slowly varying factor in the energy dependence of the relaxation time for mixed scattering has been taken as a constant over the range of integration, being designated by the symbol β in Eqs. (1), (2), and (6). It has been pointed out that this can lead to difficulties as one goes to lower temperatures and higher impurity concentrations so that the term in question ceases to be slowly varying.¹⁶ More recently, quantitative investigations of impurity mobility, in-

¹⁴ B. Abelès and S. Meiboom, Phys. Rev. **95**, 31 (1954).

¹⁵ M. Shibuya, Phys. Rev. **95**, 1385 (1954).

¹⁶ See reference 11, p. 33.

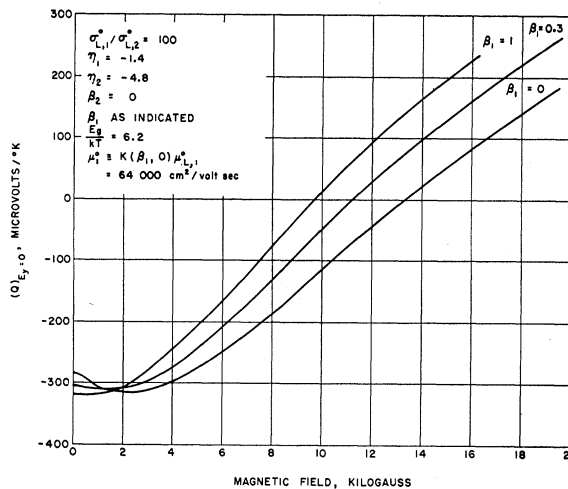


FIG. 4. Thermomagnetic effect (zero transverse electric and thermal gradients) for various degrees of electron-ion scattering.

cluding the implications of the Born approximation, which is the basis of the Conwell-Weisskoff and Brooks-Herring equations, have been carried out by Sclar¹⁷ and Blatt.¹⁸

The method employed here to evaluate the transport integrals, namely, that of replacing the slowly varying term by a constant, appropriately chosen, is discussed by Dingle¹⁹ and by Mansfield,²⁰ and applied to magnetoresistance in germanium by Willardson and Beer.²¹ The procedure is to determine this constant by using that value of the variable for which the remaining integrand assumes a maximum value (Mansfield and others) or by using a value which, when applied as a cutoff, gives a median value for the integral (Dingle). It is readily established then that the factor β is related to the lattice and impurity mobilities²² as follows:

$$\beta = 6(\mu_L^0 / \mu_I^0) [g(\bar{x}) / g(\bar{x}_I)], \quad (16)$$

where $g(x)$ is the slowly varying factor in the integrand and \bar{x} , which depends in general on β and on γ , is that value of x for which the integrand, with the g function a constant, is a maximum or which when used as a cutoff limit causes the integral to assume a median value. The argument \bar{x}_I is the value of \bar{x} for the $K(\beta, 0)$ function in the case when impurity scattering only occurs, i.e., $\beta \rightarrow \infty$. The criterion that the integrand be a maximum yields $\bar{x}_I = 3$.

The approximation in Eq. (4) is therefore to neglect the deviation of $g(\bar{x}) / g(\bar{x}_I)$ from unity. This has been done in the calculations for Figs. 1 to 4. However, as

¹⁷ N. Sclar, Bull. Am. Phys. Soc. Ser. II, **1**, 48 (1956); Phys. Rev. **104**, 1548 (1956).

¹⁸ F. J. Blatt, Bull. Am. Phys. Soc. Ser. II, **1**, 48 (1956), also **1**, 331 (1956); J. Phys. Chem. Solids **1**, 262 (1957).

¹⁹ R. B. Dingle, Phil. Mag. **46**, 831 (1955).

²⁰ R. Mansfield, Proc. Phys. Soc. (London) **B69**, 862 (1956).

²¹ R. K. Willardson and A. C. Beer, Bull. Am. Phys. Soc. Ser. II, **2**, 142 (1957).

²² It is to be noted that Mansfield's σ_I is so defined that his μ_I^0 differs from ours by the factors $g(\bar{x}_I) / g(\bar{x})$.

Mansfield points out, \bar{x} is actually a function of μ_L^0/μ_I^0 and is different for $K(\beta,0)$ and $L(\beta,0)$. In the general case considered here where $\gamma \neq 0$, Eq. (16) is still applicable although the determination of \bar{x} is more complicated since it is also a function of γ .

Finally, in very high mobility semiconductors, even moderately strong magnetic fields can lead to $\omega_0\tau$ values²³ such that the applicability of the usual Boltzmann theory treatment is in question, and effects such as electron orbit quantizations should probably be considered.²⁴ This has been discussed by Swanson²⁵ in connection with the saturation Hall constant and by Argyres and Adams²⁶ for magnetoresistance.

In conclusion, calculations made by using the mixed-scattering transport integrals should yield better results than those based on a single scattering process in such cases where scattering by acoustical phonons and ionized impurities occurs. However, the limitations of the treatment must always be kept in mind.

V. ACKNOWLEDGMENTS

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VI. APPENDIX

1. *Method of computation.*—The basis of the computations is Simpson's rule:

$$\int_0^{nh} y dx = \frac{1}{3}h(y_0 + 4y_1 + 2y_2 + 4y_3 + \dots + 2y_{n-2} + 4y_{n-1} + y_n). \quad (\text{A-1})$$

A digital machine program was set up to calculate (A-1) automatically, given n and h .

In order to determine an upper limit of integration, nh , such that truncation error might be neglected, the integrands of (1), (2) were written, respectively, as follows:

$$xe^{-x} \left(1 + \frac{\beta}{x^2} + \frac{\gamma x}{x^2 + \beta}\right)^{-1}, \quad \frac{2}{\sqrt{\pi}} x^{\frac{1}{2}} e^{-x} \left(1 + \frac{2\beta}{x^2} + \frac{\beta^2}{x^4} + \frac{\gamma}{x}\right)^{-1}.$$

For $x > 10$, the numerical value of each of these expressions is less than that of xe^{-x} . Thus, for $a > 10$, integrals

²³ Note that γ was defined on the basis of lattice scattering only and it is therefore usually larger than $\omega_0\tau$, depending on the value of β .

²⁴ Willardson, Harman, Choquard, and Beer, Phys. Rev. **98**, 227(A) (1955).

²⁵ J. A. Swanson, Phys. Rev. **99**, 1799 (1955).

²⁶ P. N. Argyres and E. N. Adams, Bull. Am. Phys. Soc. Ser. II, **1**, 298 (1956); Phys. Rev. **104**, 900 (1956).

(1) and (2) over the range a to ∞ are each less in value than

$$\int_a^\infty xe^{-x} dx = e^{-a}(1+a). \quad (\text{A-2})$$

For $a=25$, the latter expression has approximate value 4×10^{-10} . That is, the error generated in integrating (1) and (2) from zero to 25 instead of to ∞ is less than 10^{-9} . Since this is small in comparison to unit values of quoted results, $nh=25$ was taken as the upper limit in all evaluations of (A-1). The adequacy of this range was checked by calculating (A-1) for a few boundary combinations of β, γ over the range 0-50. Results agreed to at least seven significant places.

To determine the minimum number of intervals, n , into which the range of integration should be divided to provide 5-decimal accuracy, the following rule was used²⁷:

"An integral calculated by Simpson's rule using K equal intervals is correct to as many decimal places as it agrees with the same integral calculated for $2K$ equal intervals."

Preliminary machine calculations of (A-1) for numerous boundary combinations of β, γ were made to determine the minimum number of intervals necessary to give results stable to 5 decimal places or to at least 4 significant places. It was found that, depending on β and γ , between 200 and 1000 intervals were required. Final calculations were based on these minima. Quoted values are calculated values rounded to five significant places. Therefore, there may be occasional errors in the fifth significant place where more than five decimals are indicated in the tables.

2. *Details of computing process.*—Because of the similarity of Eqs. (1) and (2), both were calculated on a single machine run. The machine program and all relevant constants including all β, γ were read into machine memory by means of punched cards. The program then caused the machine to select a combination of β, γ for calculating (A-1).

To calculate each y_p of (A-1), an x_p was first calculated as

$$x_p = ph. \quad (\text{A-3})$$

The values x_p, β, γ were then used to calculate

$$y_p = x_p e^{-x_p} \left(1 + \frac{\beta}{x_p^2} + \frac{\gamma x_p}{x_p^2 + \beta}\right)^{-1}, \quad (\text{A-4})$$

and

$$y_p = x_p^{\frac{1}{2}} e^{-x_p} \left(1 + \frac{2\beta}{x_p^2} + \frac{\beta^2}{x_p^4} + \frac{\gamma}{x_p}\right)^{-1}. \quad (\text{A-5})$$

²⁷ This follows from the usual rule [see J. B. Scarborough, *Numerical Mathematical Analysis* (Johns Hopkins Press, Baltimore, 1950), second edition, p. 178]: "If we compute the value of a definite integral using subdivisions h and recompute using twice as many subdivisions, the error in the second result will be about 1/15th of the difference of the two results."

The integer p was then examined to separate even and odd y_p of (A-4) and of (A-5); y_0 and y_n were further separated from the even y_p . The y_p of (A-4) were accumulated to give:

$$\sum \text{even } y_p, \quad (\text{A-6})$$

$$\sum \text{odd } y_p, \quad (\text{A-7})$$

$$\sum (y_0 + y_n). \quad (\text{A-8})$$

A similar accumulation was done for the y_p of (A-5). When a test of p indicated that all y_p of (A-1) had

been calculated, the accumulation (A-6) was multiplied by the factor $2h/3$. The accumulation (A-7) was multiplied by $4h/3$. These products were then added to the sum of $y_0 + y_n$ to give K . Similar steps produced $2\pi^{-\frac{1}{2}}L$.

The integrals for the thermoelectric function, $K^{(2)}(\beta, \gamma)$, were calculated in the same manner as the conductivity integrals, using 400 intervals over the range 0-25. Results agreed to five significant places with a recalculation using 400 intervals over the range 0-50.

Hall Effect in Titanium, Vanadium, Chromium, and Manganese*

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The Hall effect in Ti, V, Cr, and Mn has been measured at room temperature with fields up to 30 kilosterds. The Hall constant was positive for all of these elements. The effect is extremely small in Ti and apparently sensitive to small amounts of impurities. The results for these transition elements indicate that electrical conduction is predominantly due to hole conduction.

I. INTRODUCTION

THE complex nature of the transition elements has generally limited calculation of their band structure although some detailed calculations for copper,¹ nickel,² and iron³ have been made. Because of the approximations introduced, only qualitative comparisons with experiments can be made. Usually these calculations are extrapolated to the nonferromagnetic transition elements for purposes of discussion. The general feature is a complex $3d$ band structure with a high density of states and thus a low mobility. This result agrees with both the magnetic properties and the electronic specific heat. Electrical conduction is generally considered to arise from the $4s$ electrons because of the low mobility of the $3d$ electrons. Since the Hall effect allows estimates to be made of the number of conducting particles per unit volume and their sign, this unique measurement is useful for examining some details of the band structure.

Recent measurements in the Cu-Ni⁴ alloys and the

Co-Ni⁵ alloys have demonstrated that electrical conduction is predominantly due to the $4s$ electrons; however, the results of Armco iron⁶ indicated predominant hole conduction. The increased interest in the transition elements and the availability of pure materials led to the Hall measurements described in this paper.

A brief summary of the results for Ti, V, Cr, and Mn has been given earlier.⁶ The method of measurement is that described previously.⁵ Unless specified, the sample dimensions were 6.0 cm × 1.00 cm × 0.100 cm and carried a current from 10 to 20 amperes. Whenever possible, chemical analyses of the samples are given since some of the results may be sensitive to small impurities.

II. EXPERIMENTAL RESULTS

1. Titanium

Three titanium samples were investigated, designated below as I, II, and III. Samples I and II were obtained from a commercial bar of material. Sample I was measured after machining whereas sample II was vacuum-annealed at 600°C for two hours and slowly cooled to room temperature before measurements were made. Sample III⁷ was vacuum-annealed at 800°C for 6 hours and slowly cooled to room temperature. Considerable care was exercised to avoid contamination

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