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Ionized Impurity Scattering in Nondegenerate Semiconductors

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The treatment for the scattering by ionized impurities in a semiconductor using the partial wave technique is set up and applied using a square well for the attractive impurity and a square barrier to represent the repulsive impurity. For the case $ka \ll 1$ (where k is the wave number of the charge carriers and a is the range of the impurity potential), analytical solutions are obtained for the mobility, μ, and Hall coefficients applicable to nondegenerate semiconductors at low temperatures with high impurity content. The mean free time for scattering is a function of the parameters ka and $(\pm 2m^*q^2a/\hbar^2D)^{\frac{1}{2}}$, where q is the charge of the carrier and D is the dielectric constant. The present treatment for reasonable choices of a yields limiting laws of $\mu \propto T^{-\frac{1}{2}}N_I^{-\frac{1}{3}}$ for repulsive centers, while for attractive centers there are three possible limiting cases: $\mu_1 \propto T^{-\frac{1}{2}}N_I^{-\frac{1}{3}}$, $\mu_2 \propto T^{\frac{1}{2}}N_I^{-1}$ and $\mu_3 \to \infty$. Case 2 refers to a form of resonance scattering and case 3 is the Ramsauer effect in semiconductors. These results are markedly different from previous formulas valid for $ka \gg 1$ which yield $\mu \propto T^{\frac{3}{2}}N_I^{-1}$ for both attractive and repulsive centers.

INTRODUCTION

TWO theoretical treatments have been proposed to describe ionized impurity scattering in semiconductors, the Conwell-Weisskopf[1] (C+W) and the Brooks-Herring treatments[2,3] (B+H). In the first, a classical calculation is carried out using the Coulombic scattering cross section which is cut off at a minimum angle of scattering and at a given radial distance from the scattering center. In the second a screened Coulomb potential is used and a cross section is calculated using the Born approximation. The two methods yield for the mean free time for ionized impurity scattering:

$$\tau_{(\mathrm{C+W})} = \frac{D^2(2m^*)^{\frac{1}{2}}\mathcal{E}^{\frac{3}{2}}}{\pi q^4 N_I \ln[1+(2ka)^2(D^2\hbar^2\mathcal{E}/2m^*q^4)]}\ \mathrm{sec}, \tag{1}$$

and

$$\tau_{(\mathrm{B+H})} = \frac{D^2(2m^*)^{\frac{1}{2}}\mathcal{E}^{\frac{3}{2}}}{\pi q^4 N_I \left\{ \ln[1+(2ka)^2] - \dfrac{1}{1+1/(2ka)^2} \right\}}\ \mathrm{sec}, \tag{2}$$

where N_I is the concentration of ionized impurities; D is the dielectric constant; m^* is the effective mass of the charge carriers; q is the charge of the carriers; $\hbar$ is Planck's constant divided by 2π; $\mathcal{E}$ is the energy and ka is the product of the carrier's wave number, $=2\pi/\lambda$, and the effective distance at which the potential is cut off. (It may be shown that k is proportional to $\mathcal{E}^{\frac{1}{2}}$.) It is thus seen that the only difference between these two results is in the replacement of one logarithmic term by another which, because of the insensitiveness of these logarithmic functions to this change, are roughly equal.

It may be shown that the respective formulas have similar limits of validity. The classical calculation, from a requirement that the scattering trajectory be well defined, requires $ka \gg 1$. The Born approximation, from a requirement that the phase shift be small,[4] gives the condition

$$k \gg (m^*q^2/\hbar^2 D)\ \mathrm{cm}^{-1}. \tag{3}$$

If we insert values for these symbols, we find for representative values of a that the condition $ka \gg 1$ is also satisfied. In a semiconductor, $\bar{k}$ decreases as the temperature T decreases and, further, a decreases as the concentration of ionized impurities increases. The result is that for many concentrations of ionized impurities and ranges of temperatures where ionized impurity scattering is dominant, the available treatments are not applicable.

DETERMINATION OF CUTOFF DISTANCE

The choice of a, the potential cut-off distance, requires some discussion. (C+W) have suggested that this distance be chosen equal to one-half the average distance between neighboring impurities, i.e.,

$$a_0 = 1/(2N_I^{\frac{1}{3}})\ \mathrm{cm}. \tag{4a}$$

The argument is that each ion is considered to scatter independently of its neighbors. Thus when a charge carrier exceeds the distance of $\frac{1}{2}$ the average distance from one center, then in this approximation it is scattered by the neighboring center.[5,6] (B+H) and Dingle[7] have taken for a the Debye-Hückel screening distance which is based on the statistical behavior of the conduction charges in forming a cloud of charge of the opposite sign about the ionized center and thus "cutting off" the scattering range of the center. This leads to

$$a_1 = (Dk_0T/4\pi q^2 n)^{\frac{1}{2}}\ \mathrm{cm}, \tag{4b}$$

where the symbols have their previously defined meanings, k_0 is Boltzmann's constant and n is the con-

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[1] E. Conwell and V. F. Weisskopf, Phys. Rev. **77**, 388 (1950).
[2] H. Brooks, Phys. Rev. **83**, 879 (1951).
[3] P. P. Debye and E. M. Conwell, Phys. Rev. **93**, 693 (1954).
[4] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon Press, 1949, Oxford), second edition, p. 125.
[5] N. Sclar and J. Kaplan (to be published).
[6] The correlation between centers in scattering is estimated in a forthcoming publication and is shown to be small for most of the available semiconductors.
[7] R. B. Dingle, Phil. Mag. **46**, No. 379, 831 (1955).

centration of free charge carriers. There are difficulties with both of these choices. For a_0, the effects of screening by the charge carriers, considered in a_1, have been neglected. In addition, the choice of the factor $\frac{1}{2}$ is somewhat arbitrarily based on a square uniform array of ionized centers. If spherical symmetry is assumed, for example

$$a_2 = \left(\frac{3}{4\pi}\right)^{\frac{1}{3}} \frac{1}{N_I^{\frac{1}{3}}} \text{ cm.} \tag{4c}$$

This modification would have the effect of changing the factor from 0.50 to 0.62. A further difficulty with the (C+W) choice is the use of an average distance between scattering centers. Actually, of course, there will be appreciable deviations of the positions of the ions from the average position and[8] a value for a smaller than the average may be appropriate, i.e.,

$$a_3 = (b/2N_I^{\frac{1}{3}}) \text{ cm} \quad \text{with} \quad b<1. \tag{4d}$$

With this type of adjustable constant, b, it is pointless to distinguish between (4a) and (4c).

We now discuss the applicability of (4b). (This has been previously discussed at length by Fowler.[9]) The derivation leading to (4b) is based on calculating the atmosphere of charge about a given impurity as a function of the distance from it. It is based on the solution of Poisson's equation

$$\nabla^2\phi = -4\pi\rho/D, \quad \text{with } \rho = nq\exp(-q\phi/k_0T), \tag{5}$$

where ρ is the charge density in the vicinity of a given ionized impurity. To obtain (4b), the exponential term is expanded and only the first two terms are retained. The solution of (5) then gives a screened Coulomb potential whose characteristic distance is given by (4b). The condition for the expansion of the exponential is that

$$q\phi/k_0T \ll 1, \quad \text{with } \phi = (q/Dr)\exp(-r/a). \tag{6}$$

This condition obviously cannot be realized at sufficiently small values of r. For $r=a$, we may obtain the condition

$$\frac{q^2}{2.72Dk_0Ta} \ll 1,$$

or

$$\langle ka\rangle_{\text{Av}} \gg \frac{q}{h}\left(\frac{32\pi m^* a}{2.72}\right)^{\frac{1}{2}} = 1.36\times10^4\left(\frac{\beta a}{D}\right)^{\frac{1}{2}}, \tag{7}$$

where β represents the ratio of the effective mass of the charge carriers to the free-electron mass at rest and where $\bar{k}$, the average wave number, is obtained by weighting the wave number with the Boltzmann distribution

$$\bar{k} = \langle 2\pi/\lambda\rangle_{\text{Av}} = \frac{2\pi m^*\bar{v}}{h} = \frac{4}{h}(2\pi m^* k_0 T)^{\frac{1}{2}}$$
$$= 5.37\times10^5(\beta T)^{\frac{1}{2}} \text{ cm}^{-1}. \tag{8}$$

For representative values of $(\beta a/D)^{\frac{1}{2}}$ suitable for nondegenerate semiconductors, we find that this is a requirement for $\langle ka\rangle_{\text{Av}} \geqslant 1$.

To obtain the expression a_1 (4b), it was also necessary to neglect the interaction of the charged atmosphere about a given ionized impurity with a neighboring impurity. Thus the treatment is formally valid only when it yields screening distances that are small compared to the separation of the ionized impurities. In other words, it is valid only if it yields an a that is smaller than a_3.

We return to a discussion of the quantity b introduced in (4d). It is clear that this b is to be associated with the (C+W) choice but not with the (B+H) choice. The reason is that the quantity is associated with a characteristic distance between the impurities. The (B+H) choice, however, does not depend on the separation between the impurities (it assumes infinite dilution) and thus cannot be corrected in this way. A possibility for estimating b comes from the following point of view. A necessary condition for the semiconductor to become metallic is for the radius of the bound charge about an impurity to be equal to the characteristic distance between the ionized impurities. This happens for concentrations above a certain limiting concentration of impurity. When this occurs, metallic behavior is obtained as the bound charge is now shared with all the impurities.[10] The concentration at which this occurs is approximately given by the concentration at which the ionization energy of the impurities vanishes.

This leads to $a_3 \equiv b/2N_I^{\frac{1}{3}} = a_B$. For a_B, we take the Bohr radius in the semiconductor medium:

$$a_B = D\hbar^2/\beta mq^2 \text{ cm.} \tag{9}$$

Solving for b, we obtain

$$b = 2N_I^{\frac{1}{3}}D\hbar^2/(\beta mq^2) = 1.06\times10^{-8}N_I^{\frac{1}{3}}D/\beta. \tag{10}$$

Using the values for the critical concentration of impurities[3,11] for germanium and silicon given in Table I, we calculate values of $b=0.45_2$ for germanium and $b=0.34_3$ for silicon. In the case of indium antimonide, the experimental data for the limiting concentration are not yet available. We propose to estimate b for this material from a different point of view. Now b, roughly speaking, is a measure of the extent of ordering of the impurities in the semiconductor and this is certainly a function of the temperature at which motion of the impurities is readily available. In general, for a given crystal structure, the lower the melting temperature

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[8] Regularity in positions of the ions presumes the existence of an impurity lattice, the probabilities for which are small. (See reference 5.)

[9] R. H. Fowler, *Statistical Mechnics* (Cambridge University Press, New York, 1936), second edition, p. 269.

[10] This is a necessary and sufficient condition for an impurity band.

[11] G. L. Pearson and J. Bardeen, Phys. Rev. **75**, 865 (1949).

TABLE I. Evaluation of the quantity b, used in the determination of the effective distance between impurities.

	Concentration of impurity for metallic conduction (cm^{-3})	D, dielectric constant	β, effective mass ratio	b	$T_{\rm mp}$ melting point in °K
n(Ge)	1.5×10^{17} [a]	16	0.20	0.45_2	1210
n(Si)	1.25×10^{18} [b]	12	0.40	0.34_3	1690
n(InSb)	4.9×10^{14} [c]	16	0.020	0.67_1	800

[a] See reference 3.
[b] See reference 11.
[c] Calculated.

of the material, the more ordering will be obtained, since there will be less thermal agitation to oppose the tendency of the ionized impurities to become ordered when they are free to move. (There will be an ordering tendency arising from the mutual repulsion of the impurities from each other.) In approximation, we take[12]

$$b\propto 1/T_{\rm mp}, \tag{11}$$

where $T_{\rm mp}$ is the temperature (°K) at which the semiconductor becomes liquid. Using the b values previously obtained for germanium and silicon to evaluate the constants in Eq. (11), we thus deduce the value for InSb of $b=0.67_1$. If the above approximations are valid, we may calculate the limiting concentration of impurities needed to make n-type InSb metallic. The value obtained is $4.9\times10^{14}/\text{cm}^3$, which awaits experimental verification. To verify the above, measurements in the temperature range 1–2°K will be needed.

The point of view that we are adopting in regard to the choice of the cut-off distance is to prefer that value of a_1 or a_3 which is the smaller. It is clear that in the absence of other criteria, the one yielding the smaller value will be limiting since once the ionized impurity's charge is screened or cut off, there will be no additional screening possible for a given scattering center.

RANGE OF VALIDITY

In Fig. 1, we have plotted curves for $\langle ka_1\rangle_{\rm Av}=1$ and $\langle ka_3\rangle_{\rm Av}=1$ as a function of temperature and concentration of impurities for n-type InSb, Ge, and Si. For the computation of a_1, we have taken $n_1=N-N_C\simeq N$, where N and N_C are the concentrations of the major and compensating impurities, except at the lower temperatures when $n\gg n_1$ and the calculated $a\gg a_1$. The curve $\langle ka_1\rangle_{\rm Av}=1$ is terminated at the temperature at which $n=n_1$. It is worth noting that when n becomes small as at low temperatures or for $(N-N_C)/N_C\ll1$ (compensation) that the statistical approach leading to a_1 becomes dubious and the calculation leading to a_1 less reliable. For the computation of a_3, we have used the values of b deduced above. These curves can be used to compare the relative magnitudes of the a's. Recalling that both a_3 and a_1 are inverse functions of the concentration of impurities and that $\bar{k}$ is a function of the temperature and not the concentration, then it follows that for a given temperature the curve $\langle ka\rangle_{\rm Av}=1$ lying farthest to the left (and smaller concentration coordinate) refers to the smaller value of a. Thus we see that a_1 and a_3 are roughly of the same order of magnitude and that for germanium and silicon $a_3<a_1$ at all temperatures. In the case of InSb, $a_3<a_1$ for temperatures above 14°K while $a_1<a_3$ at lower temperatures. The space to the right of the $\langle ka\rangle_{\rm Av}=1$ curves pertains to values of N_I, T where the condition $\langle ka\rangle_{\rm Av}<1$ is satisfied, while the space to the left of these curves applies to the condition $\langle ka\rangle_{\rm Av}>1$. The dashed line plotted on these curves corresponds to the usual condition for degeneracy obtained when $k_0T\leqslant E_F$ (Fermi energy).

$$T_{\rm deg}\leqslant\frac{h^2}{2m^*k_0}\left(\frac{3n}{8\pi}\right)^{\frac{2}{3}}=4.23\times10^{-11}\frac{n^{\frac{2}{3}}}{\beta}\ \text{deg.} \tag{12}$$

According to this criterion, the space to the right of these curves refers to N_I, T values where degeneracy prevails while the space to the left refers to the classical or nondegenerate region. For the case of InSb, the $\langle ka_3\rangle_{\rm Av}=1$ curve apparently lies in the degenerate region suggesting that the present nondegenerate calculation may not be applicable.[13] To illustrate the scale of these curves, regions to the right and left of the $\langle ka_3\rangle_{\rm Av}=1$ curve have been shaded in for the germanium case. The shaded region to the left of this curve includes the N_I, T

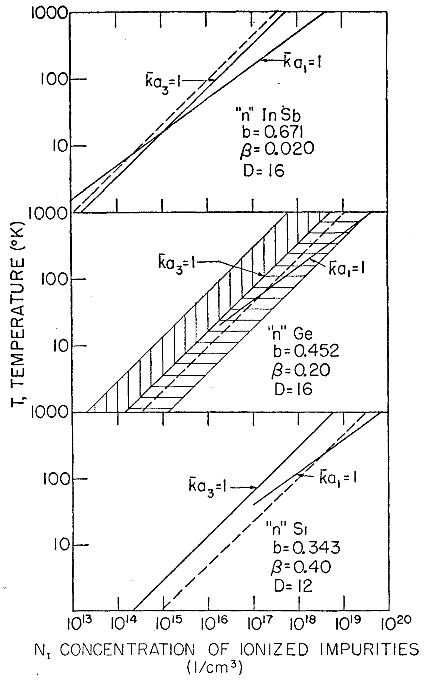

FIG. 1. Delineation of regions of validity of theory and comparison of a_3 with a_1. Here, $\bar{k}a\equiv\langle ka\rangle_{\rm Av}$ of the text.

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[12] Analysis based on a Debye-Hückel approach [Eq. (5)] with expansion of the exponential leads to this dependence.

[13] We consider degenerate cases in a future paper. Additional analysis is then necessary in making a choice of a.

for which $2 \geqslant \langle ka \rangle_{\text{Av}} \geqslant 1$ while the region to the right pertains to $\langle ka \rangle_{\text{Av}}$ values for which $1 \geqslant \langle ka \rangle_{\text{Av}} \geqslant \frac{1}{2}$. It is seen that important ranges of N_I, T values are in the $\langle ka \rangle_{\text{Av}} \sim 1$ region. For these cases numerical calculations are necessary since neither the previous treatments nor the present approximation is applicable.[5,14] There is, however, a limited range of validity for the range of $\langle ka \rangle_{\text{Av}} < 1$ which is accessible to experiment and it is of interest to obtain analytical expressions valid for this range to compare with those that are valid for $\langle ka \rangle_{\text{Av}} \gg 1$.

METHOD FOR COMPUTATION OF THE TRANSPORT PROPERTIES

To calculate the effect of ionized impurity scattering for the range $ka < 1$, we ignore the known structure of the energy bands for some of the known semiconductors and assume an isotropic quadratic energy dependence of the charge carriers on momentum. This will give rise to spherical energy surfaces in momentum space. Under these conditions, with the usual assumptions regarding the use of the Boltzmann transport equation, the mobility μ and Hall coefficient R for small magnetic fields in the extrinsic range are given, using nondegenerate statistics, by

$$\mu = \frac{4q}{3\pi^{\frac{1}{2}} m^* (k_0 T)^{5/2}} \int_0^\infty \tau \mathcal{E}^{\frac{3}{2}} \exp(-\mathcal{E}/k_0 T) d\mathcal{E}, \tag{13}$$

$$R = \frac{1}{nqc} \left(\frac{3\pi}{8} \right) \left(\frac{2(k_0 T)^{5/2}}{\pi^{\frac{1}{2}}} \right) \times \frac{\int_0^\infty \tau^2 \mathcal{E}^{\frac{3}{2}} \exp(-\mathcal{E}/k_0 T) d\mathcal{E}}{\left[\int_0^\infty \tau \mathcal{E}^{\frac{3}{2}} \exp(-\mathcal{E}/k_0 T) d\mathcal{E} \right]^2}. \tag{14}$$

The mean free time τ which is characteristic of the mechanism of scattering is given by

$$\frac{1}{\tau} = 2\pi N_I v \int_0^\pi (1-\cos\theta)[f(\theta)]^2 \sin\theta d\theta, \tag{15}$$

where $[f(\theta)]^2$ is the cross section for scattering into the angle θ and is given by[4]

$$f(\theta) = \frac{1}{2ik} \sum_{n=0}^\infty (2n+1)[\exp(2i\delta_n) - 1] P_n(\cos\theta), \tag{16}$$

where $P_n(\cos\theta)$ is the nth Legendre coefficient and δ_n is the nth phase shift which is a measure of the change in the wave function of the charge carrier induced by the scattering center. The Born approximation obtains when $\delta_n \ll 1$ and $\exp 2i\delta_n - 1 \approx 2i\delta_n$. Under this circumstance the resultant series may be summed and we obtain the familiar Born formula

$$f(\theta) = -\frac{8\pi^2 m^*}{h^2} \int_0^\infty V(r) \frac{\sin[2kr \sin(\theta/2)]}{2kr \sin(\theta/2)} r^2 dr, \tag{17}$$

where $V(r)$ is the potential characteristics of the scattering. This makes it possible to solve the scattering problem without an explicit knowledge of the phase shifts. When the Born approximation may not be made, we insert Eq. (16) into (15). After some mathematical manipulation, given in the mathematical Appendix, we obtain

$$\frac{1}{\tau} = 2\pi N_I v \frac{2}{k^2} \sum_{n=0}^\infty (n+1) \sin^2(\delta_n - \delta_{n+1}), \tag{18}$$

which is an exact expression. To proceed further it is necessary to solve the radial portion of the reduced Schrödinger wave equation

$$\frac{d^2\chi_n}{dr^2} + \left[k^2 - \frac{2m^*}{\hbar^2} V(r) - \frac{n(n+1)}{r^2} \right] \chi_n = 0. \tag{19}$$

We obtain a solution for $r < a$, and match the solution and its first derivatives to the solution obtained for $r \gg a$ at $r = a$. If γ_n is the ratio of slope to value of the interior wave function, then[15]

$$\tan\delta_n = \frac{k j_n'(ka) - \gamma_n j_n(ka)}{k\eta_n'(ka) - \gamma_n \eta_n(ka)}, \tag{20}$$

where j_n and η_n are the spherical Bessel functions and spherical Neumann functions and j_n' and η_n' are their corresponding derivatives. Thus, in principle, if we can obtain the γ_n we can solve the scattering problem. In practice, however, it is necessary to resort to numerical integration for all but the simplest scattering potentials. It is therefore of interest to ascertain how sensitive is the mean free time to the choice of scattering potential.

CHOICE OF SCATTERING POTENTIAL

To obtain information on the sensitivity of the scattering potential on the mean free time, two additional potentials were used to calcule a τ in Born approximation and these will be compared with $\tau_{(\text{C+W})}$ and $\tau_{(\text{B+H})}$. The potentials investigated were

$$V_1(r) = \begin{cases} \pm \dfrac{q^2}{D} \left[\dfrac{1}{r} - \dfrac{1}{a} \right], & r \leqslant a \\ 0, & r > a \end{cases} \tag{21}$$

$$V_2(r) = \begin{cases} \pm (q^2/Da), & r \leqslant a \\ 0, & r > a. \end{cases} \tag{22}$$

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[14] The transport properties corresponding to these cases are being calculated with the help of a digital computer.

[15] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), p. 111.

For reference we list here the potentials that lead respectively to the Conwell-Weisskopf and Brooks-Herring mean free times:

$$V(r)=\begin{cases}\pm(q^2/Dr), & \theta\geqslant\theta_{\min}=2\tan^{-1}[q^2/Dm^*v^2a_0],\\ 0 & \theta<\theta_{\min}\end{cases}\tag{23}$$

$$V(r)=\pm(q^2/Dr)\exp(-r/a_1).\tag{24}$$

Equation (21) represents a Coulomb potential which is screened by a shell of charge of opposite sign located at $r=a$. Equation (22) represents a square well or barrier potential. The results obtained using the Born approximation in a straightforward calculation, making use of the approximation that the cosine integral $\mathrm{Ci}(2ka)\simeq\sin 2ka/2ka$ for $ka\gg 1$ are

$$\tau_1=\frac{D^2(2m^*)^{\frac{1}{2}}\mathcal{E}^{\frac{3}{2}}}{\pi q^4N_I}\left(\frac{1}{[\ln(2kad)^2-1]}\right)\text{ sec},\tag{25}$$

$$\tau_2=\frac{D^2(2m^*)^{\frac{1}{2}}\mathcal{E}^{\frac{3}{2}}}{\pi q^4N_I}\left(\frac{1}{[\ln(4kad)-1]}\right)\text{ sec},\tag{26}$$

where d is a constant equal to 1.781.

Comparison with $\tau_{(\mathrm{C+W})}$ and $\tau_{(\mathrm{B+H})}$ [Eqs. (1) and (2)] indicates the mean free times are identical except for a replacement of the logarithm terms by other logarithm terms of the same order of magnitude. This result encourages us to believe that τ is indeed insensitive to the exact form of the scattering potential at least in Born approximation. To verify that this is also true for cases where $ka\lesssim 1$, we refer to the work of Morse[16] who finds that the above insensitivities carry over to these ranges as well.

PHASE SHIFT CALCULATION

Because of the above results, we take for our potential the square well or barrier potential to describe the impurities; the well describes an attractive potential while the barrier represents a respulsive potential. For this choice, analytic solutions are possible. For γ_n we have[15]

$$\gamma_n=\alpha j_n'(\alpha a)/j_n(\alpha a),\tag{27}$$

where

$$\alpha a=[k^2a^2-(2m^*V/\hbar^2)a^2]^{\frac{1}{2}}.$$

We thus see that the mean free time will be a function of the parameters ka and $[\pm(2m^*/\hbar^2)(q^2a/D)]^{\frac{1}{2}}$. Even with this simplified potential the sum of Eq. (18), is very complicated for arbitrary choices of these parameters. Since, however, this sum may be expressed in ascending powers of ka, for values of $ka<1$, it is necessary to deal with only the first few phase shifts. We work to this approximation. By making use of the properties of the spherical Bessel functions, it is possible to express Eq. (20) in the form

$$\tan\delta_n=\frac{c_n\cos ka+b_n\sin ka}{c_n\sin ka-b_n\cos ka},\tag{28}$$

where c_n and b_n are polynomials in powers of $1/ka$ and involve γ_n. After some manipulation, the quantity, $\sin^2(\delta_n-\delta_{n+1})$, which appears in our τ may then be expressed in terms of these polynomials as

$$\sin^2(\delta_n-\delta_{n+1})=\frac{(c_{n+1}b_n-c_nb_{n+1})^2}{(c_n{}^2+b_n{}^2)(c_{n+1}{}^2+b_{n+1}{}^2)}.\tag{29}$$

We list here the first few values of c_n and b_n.

$$\begin{aligned}
&c_0=1, && b_0=-(1/ka)(1+\gamma_0a),\\
&c_1=(2+\gamma_1a)/ka, && b_1=1-c_1/ka,\\
&c_2=3(3+\gamma_2a)/(ka)^2-1, && b_2=(1/ka)[3+\gamma_2a-c_2],\\
&c_3=-\frac{1}{ka}\left[3+(4+\gamma_3a)\left(1-\frac{15}{(ka)^2}\right)\right],\\
&&& b_3=-1-\frac{c_3}{(ka)^2}+\frac{5}{(ka)^2}(4+\gamma_3a).
\end{aligned}\tag{30}$$

The values of the corresponding γ_n are, from Eq. (27), if we set $x=\tan\alpha a/\alpha a$ and $z=\alpha a$:

$$\begin{aligned}
&(1+\gamma_0a)=1/x,\\
&(2+\gamma_1a)=z^2x/(x-1),\\
&(3+\gamma_2a)=(x-1)\Big/\left\{\left[\frac{3}{z^2}-1\right]x-\frac{3}{z^2}\right\},\\
&(4+\gamma_3a)=\{[3-z^2]x-3\}\Big/\left\{\left[\frac{15}{z^2}-\frac{6}{z}\right]x+\left[1-\frac{15}{z^2}\right]\right\}.
\end{aligned}\tag{31}$$

Using this formalism, we obtain respectively for attractive potentials (z real) and repulsive potentials (z imaginary) with $y=\tanh|\alpha a|/|\alpha a|$,

$$\sin^2(\delta_n-\delta_{n+1})=(ka)^2(x-1)^2[1+O(ka)^2],\tag{32a}$$

and

$$\sin^2(\delta_n-\delta_{n+1})=(ka)^2(y-1)^2[1+O(ka)^2],\tag{32b}$$

where $O(ka)^2$ means terms of the order of $(ka)^2$.

For the repulsive potentials, y is a regular monotonic decreasing function of its argument but for the case of the attractive potential the variation of the quantity x leads to two cases of interest in addition to the general case given by (32a).

Case 1.— $z\to(2n+1)\pi/2,\quad x\to\infty.$

$$\sum(0+1)\sin^2(\delta_0-\delta_1)=[1-O(ka)^2].$$

This corresponds to a resonance-type scattering.

Case 2.— $z\to\tan z;\quad x\to 1.$ (33)

$$\sum\sin^2(\delta_0-\delta_1)+2\sin^2(\delta_1-\delta_2)+3\sin^2(\delta_2-\delta_3)\simeq\tfrac{1}{3}(ka)^6[1+O(ka)^2/z^2].$$

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[16] P. M. Morse, Revs. Modern Phys. 4, 577 (1932).

This corresponds to a Ramsauer effect in semiconductors.

The corresponding mean free times for scattering are accordingly for $ka\ll 1$.

Repulsive potential.—

$$\tau_R=\frac{(2m^*)^{\frac{1}{2}}\mathcal{E}^{-\frac{1}{2}}}{8\pi N_C a^2}\left(\frac{\tanh\alpha a}{\alpha a}-1\right)^{-2}\ \text{sec},$$

where N_C is the concentration of the compensated impurity centers which give rise to repulsive centers for the free charge carriers.

Attractive potential.—

General case:

$$\tau_A=\frac{(2m^*)^{\frac{1}{2}}\mathcal{E}^{-\frac{1}{2}}}{8\pi N_A a^2}\left(\frac{\tan\alpha a}{\alpha a}-1\right)^{-2}\ \text{sec},$$

Case 1.—

$$\tau_{1A}=\frac{(2m^*)^{\frac{3}{2}}\mathcal{E}^{\frac{1}{2}}}{8\pi\hbar^2 N_A}\ \text{sec}, \tag{34}$$

Case 2.—

$$\tau_{2A}=\frac{3\hbar^4\mathcal{E}^{-5/2}}{8\pi N_A a^6(2m^*)^{\frac{3}{2}}}\ \text{sec},$$

where N_A is the concentration of attractive impurity centers.

In addition to the cases treated here, there is an additional resonance scattering condition. This obtains in the case of an attractive potential when the incident energy of the charge carrier is equal to a discrete energy associated with a bound state. For this case, $k^2=2m^*\mathcal{E}/\hbar^2$ in Eq. (19) may be replaced by $(2m^*/\hbar^2)|-\epsilon|$, where $|-\epsilon|$ is the energy of the bound state. In addition if ϵ is small enough so that we need only keep the case, $n=0$, then (19) becomes

$$\frac{d^2\chi}{dr^2}-\frac{2m^*}{\hbar^2}[\epsilon+V(r)]\chi=0, \tag{35}$$

and

$$\tau_{\text{res}}=\frac{(2m^*)^{\frac{3}{2}}(\mathcal{E}+\epsilon)}{8\pi\hbar^2 N_A\mathcal{E}^{\frac{1}{2}}}\ \text{sec}, \tag{36}$$

which is a result independent of the exact form of the potential. This expression is formally valid only for $\langle\epsilon\rangle_{\text{Av}}\simeq|-\epsilon|$. Equation (36), which we shall refer to hereafter as Case 3, should be compared with Case 1 of Eq. (34). For $\epsilon=0$, these are identical. It is unlikely that Case 3 will be important for germanium and silicon but it may be important for InSb.

In the integrals involving the μ and R, the variable $(\mathcal{E})$ is integrated between 0 and infinity.[17] The upper limit may be retained even for the range $ka\ll 1$ because $\mathcal{E}$ involves only k, so that the upper limit is still very large and may be used as infinity with little error. The lower limit in contrast with previous calculations[2] is better satisfied for this approximation. Noting that for $ka\ll 1$, $[(\tan\alpha a/\alpha a)-1]$ and $[(\tanh\alpha a/\alpha a)-1]$ are substantially independent of energy; the appropriate values for μ and R using Boltzmann statistics are in cm²/volt sec and cm³/coul, and the subscripts R and A refer respectively to the repulsive and attractive scattering:

Repulsive.—

$$\mu_R=\frac{q}{3\sqrt{2}\pi^{\frac{3}{2}}N_C a^2(m^*k_0T)^{\frac{1}{2}}}\times\frac{1}{300}\times\left(\frac{\tanh\alpha a}{\alpha a}-1\right)^{-2},$$

$$R_R=\frac{3\pi}{8}\left(\frac{1}{nqc}\right).$$

Attractive.—

$$\mu_A=\frac{q}{3\sqrt{2}\pi^{\frac{3}{2}}N_A a^2(m^*k_0T)^{\frac{1}{2}}}\times\frac{1}{300}\times\left(\frac{\tan\alpha a}{\alpha a}-1\right)^{-2},$$

$$R_A=\frac{3\pi}{8}\left(\frac{1}{nqc}\right).$$

Case 1.—

$$\mu_{1A}=\frac{4q(m^*k_0T)^{\frac{1}{2}}}{3\sqrt{2}\pi^{\frac{3}{2}}N_A\hbar^2}\times\frac{1}{300}, \tag{37}$$

$$R_{1A}=(15/16)R_A.$$

Case 2.—

$$\mu_{2A}=\frac{q\hbar^4}{(2\pi)^{\frac{3}{2}}(m^*k_0T)^{5/2}N_A a^6}\times\frac{1}{300}[-\text{Ei}(-w)]\rightarrow\infty \quad \text{as } w\rightarrow 0,$$

$$R_{2A}\rightarrow\infty \quad \text{as } w\rightarrow 0,$$

where $-\text{Ei}(-w)$ is the exponential integral

$$\textstyle\int_w^\infty[\exp(-t)/t]dt.$$

Case 3.—

$$\mu_{3A}=\mu_{1A}[1+\epsilon/(2k_0T)],$$

$$R_{3A}=R_A\left[\frac{15}{4}+6\frac{\epsilon}{k_0T}+\left(\frac{\epsilon}{k_0T}\right)^2\right]\Big/\left(2+\frac{\epsilon}{k_0T}\right)^2.$$

If we adopt a_3 to describe the cut-off distance, a, our expressions for the mobility in practical units become:

Repulsive.—

$$\mu_R=\frac{7.69\times 10^8}{N_C^{\frac{1}{3}}T^{\frac{1}{2}}\beta^{\frac{1}{2}}b^2}\left(\frac{\tanh\alpha a}{\alpha a}-1\right)^{-2}.$$

Attractive.—

$$\mu_A=\frac{7.69\times 10^8}{N_A^{\frac{1}{3}}T^{\frac{1}{2}}\beta^{\frac{1}{2}}b^2}\left[\frac{\tan\alpha a}{\alpha a}-1\right]^{-2}.$$

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[17] In the Born approximation for which $k\gg m^*q^2/\hbar^2D$, it is not formally correct to use the lower limit as zero.

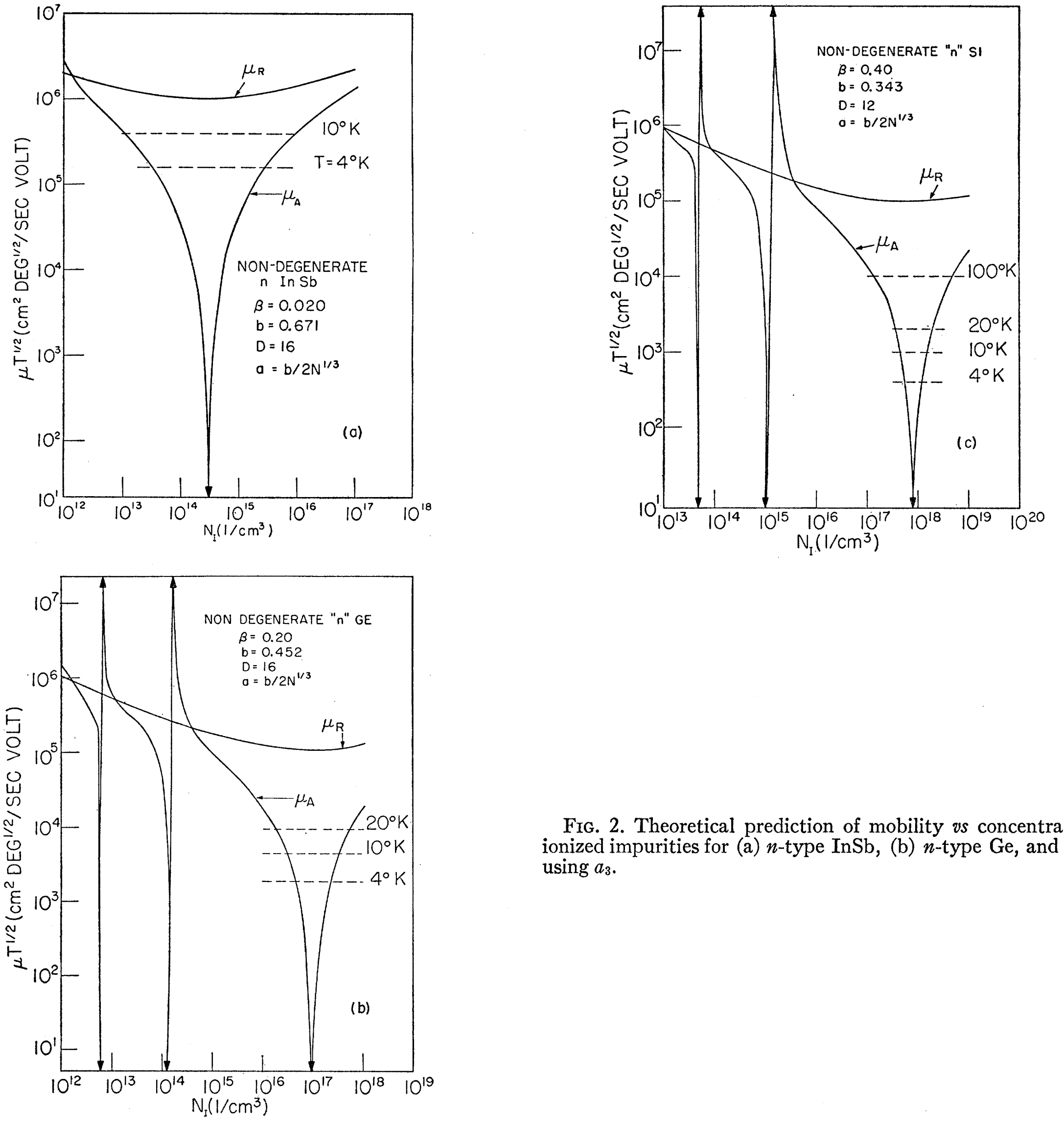

FIG. 2. Theoretical prediction of mobility *vs* concentration of ionized impurities for (a) *n*-type InSb, (b) *n*-type Ge, and (c) Si, using a_3.

Case 1.—

$$\mu_{1A}=\frac{8.68\times10^{19}\beta^{\frac{1}{2}}T^{\frac{1}{2}}}{N_A}.$$

Case 2.—

$$\mu_{2A}\rightarrow\infty. \tag{38}$$

Case 3.—

$$\mu_{3A}=\mu_{A1}[1+\epsilon/(2k_0T)],$$

with

$$\alpha a=(2m^*q^2a/\hbar^2D)^{\frac{1}{2}}=1.41\times10^4(\beta b/DN_A^{\frac{1}{3}})^{\frac{1}{2}}.$$

Since the analysis that leads to b is somewhat speculative, we list here the equations that are applicable when a_1 is used to describe the cut-off distance.

Repulsive.—

$$\mu_R=\frac{4.05\times10^6n}{D\beta^{\frac{1}{2}}T^{\frac{3}{2}}N_C}\left[\frac{\tanh\alpha a}{\alpha a}-1\right]^{-2}. \tag{39}$$

Attractive.—

$$\mu_A=\frac{4.05\times10^6n}{D\beta^{\frac{1}{2}}T^{\frac{3}{2}}N_A}\left[\frac{\tan\alpha a}{\alpha a}-1\right]^{-2}.$$

Case 1.—

$$\mu_{1A}=8.68\times10^{19}\beta^{\frac{1}{2}}T^{\frac{1}{2}}/N_A.$$

Case 2.—

$$\mu_{2A}\rightarrow\infty.$$

Case 3.—

$$\mu_{3A}=\mu_{1A}[1+\epsilon/(2k_0T)]$$

with

$$\alpha a=5.10\times10^4(\beta^2T/Dn)^{\frac{1}{4}}.$$

In view of the previous discussion of the cutoff value, we believe that for germanium and silicon, a_3 is to be preferred over equation a_1 and thus that the formulas of (38) are to be preferred over (39). Figures 2(a), 2(b), and 2(c) show a plot of $\mu T^{\frac{1}{2}}$ *vs* N_I based on formulas (38) for *n*-type InSb, Ge, and Si for the case where nondegenerate statistics are applicable. Reference should be made to Fig. 1 to determine the temperatures that are applicable. Because of the conditions $ka \ll 1$ that needs to be satisfied, the discontinuities at lower concentrations of impurities may not be realizable. The dashed curves indicate the limiting values of the mobility due to resonance scattering. The temperature dependence for the mobility is given as $\mu \propto T^{-\frac{1}{2}}$ except at resonance when $\mu \propto T^{\frac{1}{2}}$. In Fig. 3(a), we have plotted $[\mu_{\text{pw}}/\mu_{(\text{C+W},}]\{[\tan\alpha a \text{ or } \tanh\alpha a)/\alpha a]-1\}^2$ *vs* $N_I^{\frac{2}{3}}/T^2$ for *n*-type germanium where μ_{pw} is the mobility calculated here (by the partial wave technique) and $\mu_{(C+\text{W})}$ is the mobility calculated by using the Conwell-Weisskopf expression for which comparison is most readily made. This mobility is given in cm²/volt sec by

$$\mu_{(\text{C+W})} = \frac{8\sqrt{2}D^2(k_0T)^{\frac{3}{2}}}{300\pi^{\frac{3}{2}}N_Iq^3m^{*\frac{1}{2}}}\,\frac{1}{\ln[1+(3Dk_0T/q^2N_I^{\frac{1}{3}})^2]}$$
$$= \frac{3.28\times10^{15}D^2T^{\frac{3}{2}}}{\beta^{\frac{1}{2}}N_I\ln[1+3.25\times10^6(DT/N_I^{\frac{1}{3}})^2]}. \qquad (40)$$

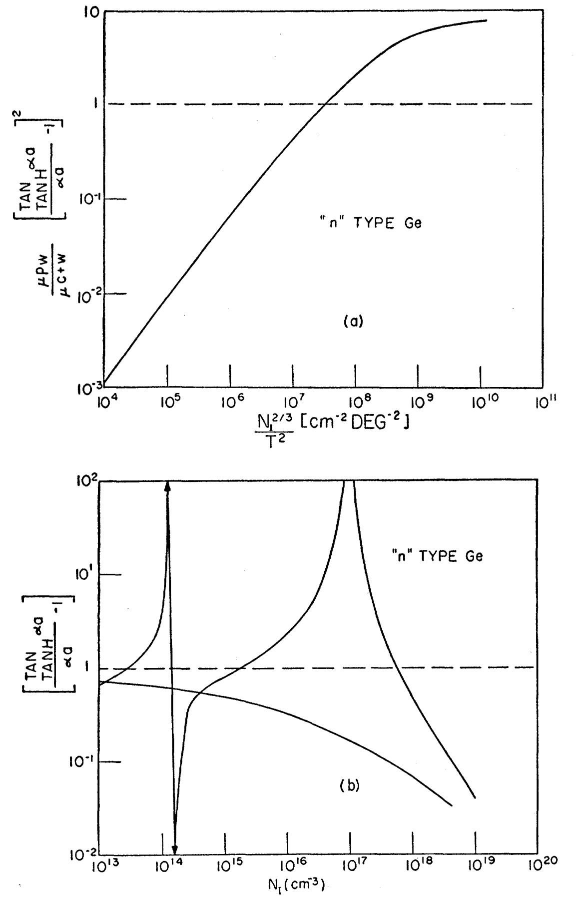

FIG. 3. Comparison of present treatment with Conwell-Weisskopf treatment.

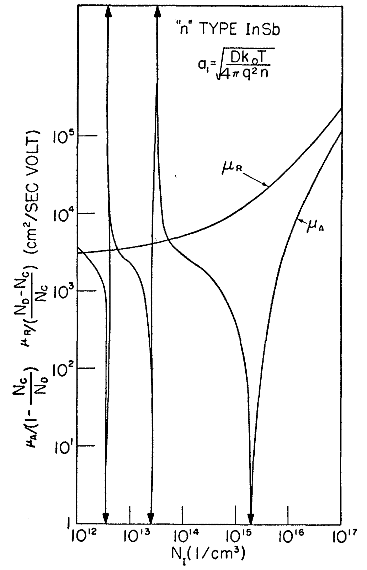

FIG. 4. Theoretical prediction of mobility *vs* concentration of ionized impurities for *n*-type InSb and Ge, using a_1 at $T=80$°K for $n \sim N_I$.

To facilitate comparison, the quantities

$$[(\tan\alpha a/\alpha a)-1]^2 \quad \text{and} \quad [(\tanh\alpha a/\alpha a)-1]^2$$

are plotted as a function of N_I in Fig. 3(b). It may be noted that for small values of $N_I^{\frac{2}{3}}/T^2$ which corresponds to low concentration and/or high temperature, the Conwell-Weisskopf calculation gives the higher value of mobility. This is also the region where $ka \gg 1$ and where the present calculation is not valid. At the higher values of $N_I^{\frac{2}{3}}/T^2$, the mobility calculated here becomes greater. This is also the range where the condition $ka \ll 1$ is more nearly satisfied. Thus, the indications are that at low temperatures and high concentrations of impurities, a higher mobility should be obtained than that predicted by the Conwell-Weisskopf (and Brooks-Herring) formula.

In Fig. 4, we have plotted the mobility as a function of the concentration of impurities when it is appropriate to use a_1 to describe the cut-off distance. This has been done for the case of InSb at 80°K. The dependence on N_I comes almost entirely from the transcendental factor since in the mobility expressions of Eq. (39) for the repulsive and attractive scattering the quantities $n/N_C = (N-N_C)/N_C$ and $n/N_A = (1-N_C/N)$ are only slightly sensitive to the concentration of the respective impurity centers. The temperature dependence is here given by a power of T that ranges between $+1/2$ and $-5/2$.

In the Conwell-Weisskopf formalism, the condition for the expansion of the logarithm term

$$(\text{i.e., } (3Dk_0T/q^2N_I^{\frac{1}{3}})^2 \ll 1)$$

is equivalent to a requirement that the minimum angle for scattering must be greater than 90°, an unrealistic condition for a classical calculation. The aforementioned requirement that $ka \gg 1$ also militates against this expansion, as may be seen in the alternate form for the logarithm term in Eq. (1). If we formally expand the logarithmic term, however, we obtain

$$\tau_{(\mathrm{C+W})}{}' = \frac{(2m^*)^{\frac{1}{2}} \mathcal{E}^{-\frac{1}{2}}}{4\pi N_I a^2} \text{ sec.} \tag{41}$$

Comparison with Eq. (34) indicates that the correct limiting functional dependence is obtained in this way with the neglect of the transcendental term of Eq. (34). Equation (41) is also greater by a factor of two. The origin of this factor of two is uncertain. It may be shown that it is not due to our use of a potential that is too small since any increased scattering tends to diminish τ rather than to increase it.

OTHER SCATTERING MECHANISMS

The other forms of scattering which may influence the mobolity are lattice vibrations, dislocations, and neutral impurity scattering. These are discussed briefly in reference 3.

The existing analyses indicate that neither lattice scattering[18] nor scattering by dislocations[19] in good[20] crystals is likely to be important at the low temperatures and the fairly high impurity concentrations for which we may expect the present theory to have applicability. On the other hand, comparison with the scattering by neutral impurities indicates that neutral impurity scattering may be comparable or dominant if N_N, the concentration of neutral impurities, is equal to or greater than the concentration of ionized impurities. Thus it is important to be able to separate the contributions of each from the experimental data or to combine the contributions of both to compare with the experimental data. In principle, this latter can be done by adding the reciprocals of the respective τ for each type of scattering and then carrying out integrals of the type of Eqs. (13) and (14) for the combined scattering. In practice, this is difficult because of the different energy dependences of the τ and a useful approximation (which however may be in error by 50% or more) is to add the reciprocals of the mobilities:

$$1/\mu = (1/\mu_I) + (1/\mu_N), \tag{42}$$

where μ_N is the mobility of the charge carriers scattered by neutral impurities. This mobility has been calculated by Erginsoy[21] and by Sclar[22] who used different models to represent the impurity. They obtain, respectively in practical units:

$$\mu_N = 1.43 \times 10^{22} \beta / D N_N, \tag{43}$$

and

$$\mu_N = 1.17 \times 10^{22} \frac{\beta}{D N_N} \left[0.734 \times 10^{-2} \frac{D T^{\frac{1}{2}}}{\beta^{\frac{1}{2}}} + 30.2 \frac{\beta^{\frac{1}{2}}}{D T^{\frac{1}{2}}} \right]. \tag{44}$$

These results, which are remarkably similar and between which it may be difficult to choose experimentally, introduce additional error in attempts to separate out the effects of neutral and ionized impurity scattering.

To complete the discussion, it is necessary to know the magnitudes of N_N, N_I, N_A, N_C, N, and n which again are respectively the concentrations of neutral impurities, ionized impurities, attractive ionized impurities, repulsive compensating ionized impurities, total major impurities and free charge carriers. The quantities are interrelated as follows: For neutral impurities, we have

$$N_N = N - N_C - n(T). \tag{45}$$

In the case of ionized impurities, when the sign of the charge associated with the ionized impurity is significant,

$$N_I = N_A = N_C + n(T) \tag{46}$$

for attractive scattering and

$$N_I = N_C \tag{47}$$

for repulsive scattering. When the scattering is independent of the sign of the charge of the impurity, as at high temperatures,

$$N_I = N_A + N_C = 2N_C + n(T). \tag{48}$$

For the case where the concentrations of free charge carriers are due to ionization from the ground state of the impurities with activation energy, $\mathcal{E}_i$,

$$\frac{(n)(N_C + n)}{N - N_C - n} = K; \quad K = \left(\frac{2\pi m^* k_0 T}{h^2} \right)^{\frac{3}{2}} \exp\left(\frac{-\mathcal{E}_i}{k_0 T} \right). \tag{49}$$

Solving for n, we obtain

$$n = -\left(\frac{N_C + K}{2} \right) \pm \left(\frac{N_C + K}{2} \right) \left[1 + \frac{4K(N - N_C)}{(N_C + K)^2} \right]^{\frac{1}{2}}. \tag{50}$$

We may expand the radical and obtain,

for low temperature:

$$K \ll N_C, \quad n \simeq [(N - N_C)/N_C] K, \tag{51}$$

for high temperature (saturation):

$$K \gg N_C, \quad n \simeq N - N_C.$$

The appropriate quantities needed for comparison with theory may thus be obtained from a measurement of the Hall coefficient since the theory indicates that $R = 1/nqc$ within a few percent except at resonance. From a knowledge of n as a function of temperature and the above relations, we can deduce the appropriate concentrations.

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[18] J. Bardeen and W. Shockley, Phys. Rev. **80**, 72 (1950).

[19] D. L. Dexter and F. Seitz, Phys. Rev. **86**, 964 (1952).

[20] By good crystals, we mean single crystals of the degree of perfection possible for well-grown germanium crystals. These are characterized by about 10^4 dislocation lines/cm^2.

[21] C. Erginsoy, Phys. Rev. **79**, 1013 (1950).

[22] N. Sclar, Phys. Rev. **104**, 1559 (1956), following paper.

DISCUSSION

It has not yet been possible to check this theory with experiment. The reason for this is that it is not easy to separate out the effects of the other mechanisms for scattering. The chief other mechanism is, as previously noted, neutral impurity scattering. Neutral impurity scattering can be reduced by the choice of material highly compensated with minority impurities [see Eq. (45)]. Previous published measurements at low temperature, however, have dealt largely with material in which attempts were made to minimize compensation. In addition, it is important to be able to determine N_C, but this requires careful measurements over a large range of temperature. In the case of n-type InSb, for which the ionization energy of impurities is small, there will be no neutral impurity scattering at low temperatures (down to about 1–2°K). Measurements on this material at low temperatures would be helpful to compare with the above theory. Because of the low degeneracy concentration in this material, the theory pertinent to the degeneracy condition will also be necessary.

In the absence of a detailed comparison with experiment, some trends of this calculation may be noted which are in agreement with experiment. These may be listed as follows:

(1) A higher mobility than given by the Conwell-Weisskopf theory is obtained at low temperature.[3]

(2) Under certain conditions, it is possible to obtain a mobility which increases as the impurity content is increased.[23,24]

(3) Under certain conditions, it is possible to obtain a mobility which is suddenly substantially reduced as the impurity content is altered.[23,24]

In addition to the details of the calculation already pointed out above, we note further that although the theory predicts a mobility that approaches infinity for scattering from attractive centers under certain conditions, this obviously is never realized. (This corresponds to the Ramsauer effect in semiconductors.) The reason is twofold. We have taken for a an average value to describe the range of the scattering potential. Fluctuations from this average will give rise to deviations from the extreme condition. The second reason is that the other mechanisms for scattering, i.e., lattice, neutral impurities, or repulsive ionized impurities, take over and limit the mobility. In the other extreme (resonance scattering), the mobility is prevented from reaching zero by the details of the calculation (Case 2) which limit the scattering. An important aspect of this calculation compared with previous calculations is that there is a fundamental difference between scattering from a repulsive center and an attractive center. We can see why this is so from an intuitive argument. For high-energy particles there is little chance for a particle to be bound. We therefore expect equal deviations to be caused in the path of a particle scattering from an impurity although the deviations will be in opposite directions. In the case of low-energy particles, however, where there is a chance that a particle of the proper sign may be bound, we would expect an appreciable difference between the impurity centers since an attractive impurity may swing the particle into an orbit about it, whereas a repulsive impurity would merely scatter in the usual way.

The present calculation suffers from the following defects:

(1) It is limited to the range $ka \ll 1$.

(2) Polarization and exchange effects have been neglected throughout. These effects are quite important with neutral centers at low particle velocities, but for the ionized scattering considered here they are negligible because it is unlikely that we can produce a polarization in the impurity that can be comparable with the Coulombic force already present, and in the case of exchange, no exchange is possible (in first approximation) because of the tight binding of the electrons in the filled shells of the impurities.

(3) We have ignored impurity band conduction since this is not yet well established, and the phenomenon may in fact be due to the effects described here.

(4) No account has been taken of the known structure of the energy bands. It is known that when this effect is taken into account it alters some of the details of the calculation. For the n-type material considered here, the effect (ellipsoidal energy surfaces) may be to change the definition of the effective mass if the scattering between surfaces is ignored.

Although these calculations are applicable only for $ka \ll 1$, it is possible to visualize the pattern to be expected as $ka \rightarrow 1$. Inspecting the expression for αa [Eq. (27)], we note that it is symmetrical in both ka and $[(2m/\hbar^2)V]^{\frac{1}{2}}a$. Thus, we can expect a type of resonance condition in τ for ka similar to those obtained for $(2m/\hbar^2 V)^{\frac{1}{2}}a$ for particular values of this parameter. The resulting effect on the mobility and Hall coefficient will be somewhat different from that obtained here because of the weighting and integration with $\mathcal{E}$ required. However, there nevertheless exists a possibility of explaining the anomalous behavior of the Hall coefficient and magnetoresistance in germanium as a function of temperature in the low-temperature range.[24] Previously this behavior has been attributed to a property of an impurity band but such an explanation does not seem able to explain all of the experimental findings. It is hoped that the numerical calculation being performed that will cover this range, will be able to elucidate this question.

Note added in proof.—In addition to the potential cut-off distances considered in Eq. (4), at low temperatures when $n \ll N_C$ and a_1 [Eq. (46)] fails, another choice is possible. This is a_1 with n replaced by N_C. This possibility arises from the preferential population-

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[23] F. J. Morin and J. P. Maita, Phys. Rev. **96**, 28 (1954).

[24] H. Fritzsche, Phys. Rev. **99**, 406 (1955).

ing of the neutral centers by the free charge carriers in such a way that the remaining attractive ionized centers are effectively screened by the compensating ionized impurities. I am indebted to Dr. G. R. Gunther-Mohr for pointing out this additional possibility.

APPENDIX I. DERIVATION OF EQ. (18)

We have

$$\frac{1}{\tau}=2\pi Nv\int_0^\pi (1-\cos\theta)[f(\theta)]^2\sin\theta d\theta, \tag{A1}$$

with

$$f(\theta)=\frac{1}{2ik}\sum_{n=0}^{\infty}(2n+1)[\exp(2i\delta_n)-1]P_n(\cos\theta). \tag{A2}$$

Squaring (2) gives

$$[f(\theta)]^2=\left[\frac{1}{2k}\sum_{n=0}^{\infty}(2n+1)(\cos2\delta_n-1)P_n(\cos\theta)\right]^2+\left[\frac{1}{2k}\sum_{m=0}^{\infty}(2m+1)\sin2\delta_m P_m(\cos\theta)\right]^2$$

$$=\frac{1}{4k^2}\left\{[\sum_{l=0}^{\infty}(2l+1)]^2 2(1-\cos2\delta_l)P_l^2(\cos\theta)+\sum_{m,n\,(m\neq n)}^{\infty}(2n+1)(2m+1)\right.$$
$$\left.\times[(\cos2\delta_n-1)(\cos2\delta_m-1)+\sin2\delta_n\sin2\delta_m]P_nP_m\right\}.$$

Collecting terms and making use of trigonometric identities, we obtain

$$[f(\theta)]^2=\frac{1}{4k^2}\left\{[\sum_{l=0}^{\infty}(2l+1)^2 4\sin^2\delta_l P_l(\cos\theta)+2\sum_{n,m\,(n<m)}(2n+1)(2m+1)[4\sin^2\delta_n\sin^2\delta_m+\sin2\delta_n\sin2\delta_m]P_nP_m\right\}.$$

Let

$$I=\int_0^\pi [f(\theta)]^2(1-\cos\theta)\sin\theta d\theta,\quad x=\cos\theta;$$

then

$$dx=-\sin\theta,\quad \int_0^\pi=\int_{+1}^{-1}=-\int_{-1}^{1}$$

and

$$I=\frac{1}{4k^2}\int_{-1}^{1}\left\{\sum_{l=0}^{\infty}(2l+1)^2 4\sin^2\delta_l P_l^2(x)+2\sum_{n,m\,(n<m)}(2n+1)(2m+1)[4\sin^2\delta_n\sin^2\delta_m+\sin2\delta_n\sin2\delta_m]P_nP_m\right\}(1-x)dx$$

$$=\frac{2}{k^2}\left\{\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l-\sum_{n=0}^{\infty}(n+1)[2\sin^2\delta_n\sin^2\delta_{n+1}+\tfrac{1}{2}\sin2\delta_n\sin2\delta_{n+\cdot1}]\right\},$$

where we have used the integral properties of the Legendre polynomials. Using again trigonometric identities and combining the running indices, we obtain

$$I=\frac{2}{k^2}\left\{\sum_{n=0}^{\infty}(n+1)[\sin^2\delta_n\cos^2\delta_{n+1}+\sin^2\delta_{n+1}\cos^2\delta_n-2\sin\delta_n\cos\delta_n\sin\delta_{n+1}\cos\delta_{n+1}]+\sum_{n=0}^{\infty}n\sin^2\delta_n-(n+1)\sin^2\delta_{n+1}\right\}.$$

But

$$\sum_{n=0}^{\infty}n\sin^2\delta_n-(n+1)\sin^2\delta_{n+1}=0,$$

as may be seen by writing the terms down and canceling the $(n+1)$ terms with the n terms. Thus

$$I=\frac{2}{k^2}\sum_{n=0}^{\infty}(n+1)\sin^2(\delta_n-\delta_{n+1}),$$

upon using a trigonometric identity, and

$$\frac{1}{\tau}=(2\pi N_I v)\frac{2}{k^2}\sum_{n=0}^{\infty}(n+1)\sin^2(\delta_n-\delta_{n+1}),$$

which is Eq. (18).