Stopping Power of L-Electrons*

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The Bethe theory of the energy loss of fast charged particles is extended to treat explicitly the stopping contribution of L-shell electrons. A summary of the effect of binding corrections on stopping power is given.

I. INTRODUCTION

CCORDING to Bethe's^{1,2} theory on the energy loss of charged particles passing through matter, the energy loss per cm path length is

$$-\frac{dE}{dx} = \frac{4\pi e^4 z^2}{mv^2} NB,\tag{1}$$

with the so-called stopping number, $B = Z \ln(2mv^2/I)$. For the stopping atoms, N is the number per cm³, Z the atomic number, and I the average ionization potential; for the incident particle, ez is the charge and v the velocity. m is the electronic mass.

Equation (1) is valid without correction for the binding effects of the atomic electrons only if the velocity of the incident particle is much greater than the "velocity" of the atomic electrons. When this is not so, the contribution to B from these electrons must be calculated separately, and in a way free from the approximations which limit (1). Using hydrogenic wave functions, Bethe² has done this for the contribution from the K-shell electrons, B_K . Revised curves of B_K vs η_K for various Z are given in Fig. 1 of a previous paper (K).3 η_K is a convenient variable given as a quotient of $mv^2/2$ by the "ideal" ionization potential, $Z_{K \text{ eff}}^2 R_H$ (R_H is the ionization potential of the hydrogen atom). In K, the work of Brown⁴ is also extended and corrected to provide an asymptotic expression for B_K for large η_K of the form⁵

$$B_K(\theta_K, \eta_K) = S_K(\theta_K) \ln \eta_K + T_K(\theta_K) - C_K(\theta_K, \eta_K), \quad (2)$$

where θ_K is the observed ionization potential (more accurately the energy difference between ground state and lowest unoccupied state) in units $Z_{K \text{ eff}^2} R_H$. Curves of C_K vs $1/\eta_K$, over the range $0 \le 1/\eta_K \le 2$, for various θ_K , hence Z, are given in Fig. 2 of K. Obviously, given B_K , S_K and T_K , C_K is determined for η_K large or small. Thus C_K may be extended to larger $1/\eta_K$ $(\eta_K < \frac{1}{2})$ by

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tion of Charged Particles in Matter.

¹ H. A. Bethe, Ann. Physik 5, 325 (1930).

² M. S. Livingston and H. A. Bethe, Revs. Modern Phys. 9,

263 (1937).

³ M. C. Walske, Phys. Rev. 88, 1283 (1952), referred to hereafter as K.

L. M. Brown, Phys. Rev. 79, 297 (1950).

using the B_K curves of K, and formula (2) above. For the region of small $1/\eta_K$ ($\eta_K > 10$, say), C_K may best be determined from its expansion in powers of $1/\eta_K$,

$$C_K(\theta_K, \eta_K) = U_K(\theta_K) \eta_K^{-1} + V_K(\theta_K) \eta_K^{-2} + \cdots, \quad (3)$$

where U and V are given in formula (19) of K.

In K, formulas (2) and (3) above are generalized for any atomic shell i, and the total stopping number B is written

$$B = Z \ln(2mv^2/I) - \sum_i C_i(\theta_i, \eta_i),$$

with I, the average ionization potential, defined in a way independent of the velocity of the incident particle. This formulation demonstrates the usefulness of C_i as opposed to B_i . C_i provides the simplest way of correcting the stopping number B of formula (1) for the so-called binding effects.

In this paper, we shall extend the theory to include corrections for L-shell electrons. First we shall calculate B_L for the L-electrons, giving curves of B_L vs η_L in Fig. 2. We then calculate θ_K^{7} and θ_L for various Z, presenting the results in Fig. 1. The constants S_L , T_L , and U_L are then found so that C_L is determined for all η_L . The resulting asymptotic calculation for C_L is checked for several large values of η_L by comparing its results with those from an exact calculation. Finally a summary is given of the total effect of K- and L-shell binding corrections on stopping power.

II. CALCULATION OF $B_L(\theta_L, \eta_L)$

Using formula (5) of K, we can write an expression for the stopping number of the L-shell which is not restrictive on the velocity of the incident particle:

$$B_{L}(\theta_{L},\eta_{L}) = \int_{W_{\min} = \theta_{L}/4}^{\infty} WdW \times \int_{W/(4\eta_{L})^{\frac{1}{2}}}^{\infty} \frac{2dq}{q^{3}} |F_{W,L}(q)|^{2}, \quad (4)$$

where W is the energy transferred to the atomic electron in units⁸ $Z_{L \text{ eff}^2} R_{\text{H}}$, q = (change in incident particle's)momentum)/ $(2mZ_{L \text{ eff}}^2 R_H)^{\frac{1}{2}}$, and $|F_{W,L}(q)|^2$, the socalled form factor, is the sum of the squares of the

⁵ This is an asymptotic expression since C_K approaches zero as η_K approaches infinity.

⁶ S and T are given in formula (19) of K.

⁷ It would have been better to have included θ_K is Z in K.
8 Z_L off may be taken as Z-4.15, following J. C. Slater, Phys. Rev. 36, 57 (1930).

ηL	W = 0.09	0.11	0.1389	0.1875	0.25	0.3611	0.50	0.8125	1.25	2.5	4.25	9.25	16.25
0.1	475	282	156	69.2	30.8	9.0	2.20	0.10	0.0047	(1 \ 110 - 8	0.01440-8		
0.1	832	498	277	129.2	63.0	$\frac{8.9}{24.8}$	2.28 10.0	$0.12 \\ 1.68$	$0.0045 \\ 0.126$	6.1×10 ⁻⁶	2.3×10 ⁻⁸		
0.3	1088	653	359	166.7	82.2	33.6	14.9	3.97	0.120	2.9×10^{-4} 3.5×10^{-3}	1.3×10^{-6} 1.4×10^{-5}		
0.4	1306	776	421	193.3	94.6	38.9	17.84	5.42	1.50	2.0×10^{-2}	9.2×10 ⁻⁵		
0.5	1492	877	470	213.8	104.0	42.5	19.64	6.25	2.07	7.5×10^{-2}	4.3×10 ⁻⁴		
0.6	1657	963	512	230.4	110.8	45.1	20.85	6.74	2.42	0.190	1.6×10 ⁻³		
0.7	1799	1038	546	244.2	116.7	47.1	21.74	7.09	2.62	0.330	4.9×10^{-3}		
0.8	1928	1104	578	256.1	121.6	48.8	22.42	7.33	2.76	0.451	1.4×10^{-2}	1.9×10 ⁻⁶	
0.9	2044	1164	606	266.4	125.8	50.1	22.98	7.50	2.85	0.534	3.2×10^{-2}	4.0 × 10 −6	
1.0	2149	1218	630	275.7	130.2	51.3	23.44	7.64	2.91	0.588	6.1×10^{-2}	9.1×10^{-6}	
1.1	2247	1268	653	284.0	133.6	52.3	23.82	7.76	2.96	0.624	9.7×10^{-2}	2.0×10^{-5}	
1.25	2379	1335	684	295.0	137.3	53.6	24.31	7.88	3.01	0.655	0.148	5.8×10 ⁻⁵	
1.5	2572	1432	727	310.9	142.9	55.4	24.95	8.04	3.07	0.682	0.198	3.2×10^{-4}	
1.75	2738	1516	765	324.0	147.8	56.8	25.44	8.15	3.11	0.695	0.218	1.5×10^{-3}	
2.0	2886 3133	1589 1714	797 951	335.3	152.0	58.0	25.84	8.24	3.13	0.703	0.227	5.9×10^{-3}	2.3×10^{-6}
2.5 3.5	3515	1899	851 932	354.1 382	158.9 168.8	59.9 62.6	26.47	8.37	3.17	0.711	0.233	2.9×10^{-2}	2.2×10^{-5}
3.3	3313	1099	934	304	100.0	02.0	27.34	8.54	3.21	0.718	0.236	4.7×10^{-2}	1.2×10^{-3}

Table I. The L-shell excitation function, $J(\eta_L, W)$.

matrix elements of e^{iqx} between the four nonrelativistically distinct L-shell states and the states greater in energy by W. Analogously to η_K and θ_K , $\eta_L = mv^2/2Z_{L~{\rm eff}}^2R_{\rm H}$, and θ_L is the observed energy difference between an L-electron in the ground state and the lowest unoccupied state in units $Z_{L~{\rm eff}}^2R_{\rm H}$. The integral over W means a sum over all unoccupied discrete states, and an integration over the continuum states.

The evaluation of the form factor, $|F_{W,L}(q)|^2$, follows the analogous work of Wentzel⁹ and Bethe¹ for the K-shell. The calculation is done with nonrelativistic hydrogenic wave functions for transitions from the four distinct L-shell states to states greater in energy by W. $|F_{W,L}(q)|^2$ arises then from summing over all eight L-shell electrons and all states greater by energy W. Since the calculation is long and tedious, and since no new principles are involved, we quote only our results here:

For transitions to the continuum $(W = k^2 + \frac{1}{4})$,

$$|F_{W,L}(q)|^{2}dW = \frac{dW}{1 - e^{-2\pi/k}}$$

$$\times 2^{4}q^{2} \exp\left(-\frac{2}{k} \arctan \frac{k}{q^{2} - k^{2} + \frac{1}{4}}\right)$$

$$\boxed{[(q+k)^{2} + \frac{1}{4}]^{4}[(q-k)^{2} + \frac{1}{4}]^{4}}$$

$$\times \left[q^{6} + \left(-\frac{11}{12} - \frac{5}{3}k^{2}\right)q^{4} + \left(\frac{65}{48} + \frac{3}{2}k^{2} + \frac{1}{3}k^{4}\right)q^{2} + \left(\frac{5}{64} + \frac{23}{48}k^{2} + \frac{3}{4}k^{4} + \frac{1}{3}k^{6}\right)\right]. (5)$$

For transitions to discrete states $(W = \frac{1}{4} - 1/n^2)$, with the W subscript of F changed to n for identification,

our result is

$$|F_{n,L}(q)|^{2} = 2^{5}n^{7}q^{2}\frac{\left[\left(\frac{1}{2}n-1\right)^{2}+q^{2}n^{2}\right]^{n-4}}{\left[\left(\frac{1}{2}n+1\right)^{2}+q^{2}n^{2}\right]^{n+4}}$$

$$\times \left[q^{6}n^{6}+\left(-\frac{11}{12}n^{2}+\frac{5}{3}\right)q^{4}n^{4}+\left(\frac{65}{48}n^{4}-\frac{3}{2}n^{2}+\frac{1}{3}\right)q^{2}n^{2}+\left(\frac{5}{64}n^{6}-\frac{23}{48}n^{4}+\frac{3}{4}n^{2}-\frac{1}{3}\right)\right]. (6)$$

It is easy to show that (6) can be derived from (5) if one replaces k^2 by $-1/n^2$, and if one replaces the continuum normalization factor, $[1-\exp(-2\pi/k)]^{-1}$ by unity. For this reason it is permissible to use formula (5) in (4) even for values of W less than $\frac{1}{4}$.

We can now evaluate (4) numerically. Again we only quote results, since the details of the calculation are quite lengthy. The first step is the evaluation of

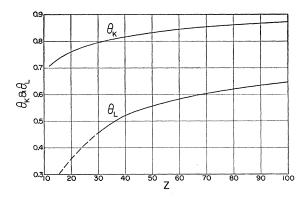


Fig. 1. θ_K and θ_L as functions of Z.

⁹ Gregor Wentzel, Z. Physik 58, 348 (1929).

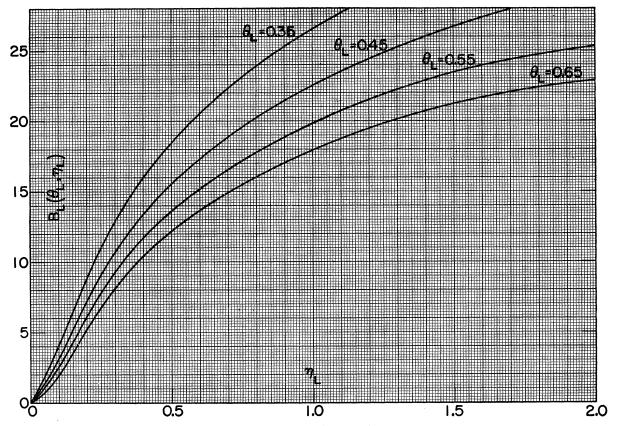


Fig. 2. $B_L(\theta_L, \eta_L)$, stopping number contribution of L-electrons.

the so-called excitation function,

$$J(\eta_L, W) = \int_{W/(4\eta_L)^{\frac{1}{2}}}^{\infty} \frac{2dq}{q^3} |F_{W, L}(q)|^2, \tag{7}$$

for the various W and η_L . The results are tabulated in Table I. Then carrying out the integration over W we obtain $B_L(\theta_L,\eta_L)$ with the results plotted in Fig. 2 for $0 \le \eta_L \le 2$, and tabulated in Table II for $1.0 \le \eta_L \le 3.5$. The numerical calculations are accurate to at least one percent. The theory, itself, due to the use of Coulomb wave functions, is probably in error by considerably more. However, the labor involved in calculating with

Table II. Stopping number contribution of L-electrons, $B_L(\theta_L, \eta_L)$.

ηL	$\theta_L = 0.35$	$\theta_L = 0.45$	$\theta_L = 0.55$	$\theta_L = 0.65$
1.0	26.52	22.48	19.80	17.89
1.1	27.70	23.48	20.70	18.71
1.25	29.32	24.86	21.95	19.87
1.5	31.48	26.68	23.56	21.36
1.75	32.89	27.79	24.51	22.20
2.0	34.09	28.74	25.31	22.90
2.5	36.88	31.09	27.40	24.84
3.5	40.34	33.87	29.81	27.01

more refined wave functions, such as Hartree's, for example, would be much greater, and such a calculation would have to be repeated for each Z.

As regards the use of our B_L results for different Z, it should be remarked that one can expect the results to be most applicable where the hydrogenic wave functions best resemble the true wave functions of the atom. This is best satisfied for the heavier elements. We shall see later that for Z < 30 ($\theta_L < 0.45$) the error associated with the use of hydrogenic wave functions makes our results unreliable. We shall propose there an alternate method for low Z (and not very low η_L).

III. CALCULATION OF θ_K AND θ_L

Hönl¹⁰ has shown that in a calculation using non-relativistic wave functions, such as ours, the best value to take for θ_i is given by

$$\theta_i = 1 - (I_{R, i} - I_{0, i}) / I_{NR, i},$$
 (8)

where $I_{R,i}$ is the "ideal" relativistic ionization potential of an i-shell electron in the absence of "outer screening," given to a good approximation for the K-electrons and for the three relativistically different L-electron states

¹⁰ H. Hönl, Z. Physik 84, 1 (1933).

by (in Rydbergs)

(K)
$$(l=0, j=\frac{1}{2})$$
 $(Z-0.3)^2\left(1+\frac{(Z-0.3)^2}{4}\alpha^2\right)$,

$$(L_{\text{III}})$$
 $(l=0, j=\frac{3}{2})$ $\frac{(Z-4.15)^2}{4} \left(1 + \frac{(Z-4.15)^2}{16}\alpha^2\right).$

 $(\alpha = 1/137)$.

 $I_{NR,i}$ is the corresponding nonrelativistic ionization potential, $(Z-0.3)^2$ for the K-electrons, and $(Z-4.15)^2/4$ for the L-electrons. $I_{0,i}$ is the observed (from the x-ray critical absorption wavelength) energy difference from the i-shell to the lowest-lying unoccupied state.

For the K-shell the evaluation of (8) is straightforward, and the results are given in Fig. 1, where θ_K is plotted vs Z. In the case of θ_L , one gets three values for each Z, corresponding to the three relativistic L-electron energy states. The values for the two p-states are generally less than one percent apart. The value for the s-state differs from those for the p-states by from five to ten percent. Therefore, in order to form a single value to use with B_L , we take an average of these three values, weighting them according to the L-shell oscillator strengths from Hönl. The resulting curve of $\theta_L vs$ Z is also given in Fig. 1.

IV. ASYMPTOTIC FORMULA FOR $B_L(\theta_L, \eta_L)$

The derivation of the asymptotic formula for $B_L(\theta_L,\eta_L)$ proceeds in a way entirely similar to that used in obtaining formula (2) for $B_K(\theta_K,\eta_K)$. This method, of course, is detailed in K which in combination with Brown's work solves the problem. Here we only summarize our results for the L-shell.

We first give a preliminary result which is $B_L(\theta_L=1, \eta_L)$, the stopping number for eight hydrogen-like *L*-electrons in a hypothetical atom with no transitions to other shells forbidden by the Pauli principle,

$$B_L(\theta_L=1, \eta_L) = 8 \ln \eta_L + 25.5166 - 2\eta_L^{-1}$$
 (to order $1/\eta_L$). (10)

Taking into account the transitions that are forbidden by the Pauli principle, and modifying (10) accordingly, we then have our desired result (to order $1/\eta_L$) for $B_L(\theta_L,\eta_L)$:

$$B_L(0.35, \eta_L) = 10.0371 \ln \eta_L + 28.1449 - 1.5032 \eta_L^{-1},$$

$$B_L(0.45, \eta_L) = 7.9116 \ln \eta_L + 24.4501 - 1.8756 \eta_L^{-1},$$

$$B_L(0.55, \eta_L) = 6.7451 \ln \eta_L + 21.9061 - 1.9890 \eta_L^{-1},$$

$$B_L(0.65, \eta_L) = 6.0345 \ln \eta_L + 20.0154 - 2.0040 \eta_L^{-1}.$$
(11)

An asymptotic formula for $C_L(\theta_L, \eta_L)$ to order η_L^{-1} is given by the negative of the last term of (11).

Table III. $C_L(\theta_L, \eta_L)$ from exact calculation.

θ_L	$\eta_L = 1$	3.5	10	25	100	1000
0.35	1.6934	0.4917	0.1619	0.06235	0.01516	0.001505
0.45	2.0298	0.5950	0.1988	0.07719	0.01888	0.001877
0.55	2.1358	0.6268	0.2100	0.08171	0.02001	0.001991
0.65	2.1519	0.6312	0.2116	0.08232	0.02016	0.002006

 $C_L(\theta_L,\eta_L)$ can be calculated exactly by using formula (8) of K, and performing the necessary numerical integration. The results are given in Table III. The last term of (11) gives results which are low by about 9, 5, 3, 0.6, and 0.08 percent at η_L =3.5, 10, 25, 100, and 1000, respectively, for θ_L =0.65. The errors are similar for other θ_L . It is possible to fit further terms in η_L^{-1} to the exact calculation. The results, numerically accurate to at least 0.2 percent for the above η_L and all θ_L , are

$$\begin{split} C_L(\theta_L = 0.35, \eta_L) &= 1.503 \eta_L^{-1} + 1.543 \eta_L^{-2} \\ &- 4.00 \eta_L^{-3} + 4.43 \eta_L^{-4}, \\ C_L(\theta_L = 0.45, \eta_L) &= 1.876 \eta_L^{-1} + 1.506 \eta_L^{-2} \\ &- 4.00 \eta_L^{-3} + 4.43 \eta_L^{-4}, \\ C_L(\theta_L = 0.55, \eta_L) &= 1.989 \eta_L^{-1} + 1.498 \eta_L^{-2} \\ &- 4.00 \eta_L^{-3} + 4.43 \eta_L^{-4}, \\ C_L(\theta_L = 0.65, \eta_L) &= 2.004 \eta_L^{-1} + 1.500 \eta_L^{-2} \\ &- 4.00 \eta_L^{-3} + 4.43 \eta_L^{-4}. \end{split} \tag{12}$$

If (11) is rewritten with the first two terms combined, ¹¹ then from the basic Bethe theory we should expect them to have the form $2mv^2/(\frac{1}{4}Z_{L\text{ eff}}^2R_{\text{H}})=16\eta_L$. If we write the actual logarithm as $\ln(16\eta_L/\lambda_L)$, we find for λ_L the values given in Table IV. ¹² It is remarkable that λ_L decreases with increasing θ_L (increasing Z). Over the range $0.45 \leqslant \theta_L \leqslant 0.65$, however, the variation is quite slow.

A simple extension of the results of reference 12 to the L-shell reveals that the coefficients of the logarithm terms in (11) are equal to $8(1+f_L)/2=4+4f_L$, where $8f_L$ is the total oscillator strength of the eight L-electrons for transitions to unoccupied states. The values of f_L obtained from these coefficients are displayed in Table IV. We also give the quantity $\theta_L^2 f_L$ whose small variation shows that for the L-shell (as for the K-shell) f_L is very nearly inversely proportional to θ_L^2 .

TABLE IV. Calculated results for the *L*-shell using hydrogenic wave functions.

θ_L	λL	f_L	$\theta L^2 f L$
0.35	0.967	1.51	0.185
0.45	0.729	0.98	0.198
0.55	0.622	0.69	0.208
0.65	0.580	0.51	0.215
Hydrogen	0.659	1	

 $^{^{11}}$ I.e., $S_L(\theta_L) \ln[\exp T_L(\theta_L)/S_L(\theta_L)]\eta_L$. 12 See Bethe, Brown, and Walske, Phys. Rev. **79**, 413 (1950) for the corresponding K-shell data.

TABLE V. Approximate percentage correction to (1) from C_K and C_L .

ncident proton energy (Mev)	Z = 30	50	70	90
1	$+4.3^{a}$	$+14^{a}$	+21 ^b	+26b
5	-3.9a	-1.4^{a}	$+ 1.4^{a}$	$+ 2.8^{b}$
10	-3.0	-2.3	-0.7^{n}	$+ 0.4^{b}$
20	-1.7	- 2.0	-1.5^{a}	- 0.9a
50	-0.9	- 1.2	- 1.3	- 1.1a
100	-0.4	-0.7	- 0.8	- 0.9
200	-0.2	-0.4	- 0.5	-0.5
500	-0.07	-0.14	- 0.2	-0.3
1000	-0.03	-0.06	- 0.09	-0.13

a For these values C_K is negative (see text). b For these values C_K and C_L are negative (see text).

A comparison of our values of f_L with those obtained by Hönl¹⁰ shows a close check as indeed it should since they were both obtained in the same approximation, i.e., using hydrogen-like wave functions. Like Hönl we observe that for $\theta_L = 0.35$ this approximation gives a value of f_L which is much too high. Since the oscillator strength per electron for hydrogen for a transition $2p \rightarrow 1s$ is $^{13} - 0.139$, we can set an upper limit for f_L of about $1 + \frac{3}{4}(0.139) \approx 1.1$. Thus we see that our calculations of B_L and C_L for $\theta_L < 0.45$ are not reliable. Lacking a more accurate calculation of an asymptotic formula for this region (Z < 30), it is reasonable to proceed as

follows: Calculate f_L using Hartree wave functions for the desired atom, and then with this f_L and a corresponding λ_L from Table IV, write $B_L \simeq 4(1+f_L) \ln(16\eta_L/\lambda_L)$.

V. SUMMARY OF EFFECT OF K- AND L-SHELL BINDING CORRECTIONS

In order to summarize the effect of the K- and L-shell binding corrections, in Table V, we give for various Z and incident proton energies the approximate percentage correction to the simple formula (1) introduced by C_K and C_L . Since the first two terms of B_K , given by (2), may be written $S_K(\theta_K) \ln\{\eta_K \exp[T_K(\theta_K)/S_K(\theta_K)]\}$, it is apparent that for $\eta_K < \exp[-T_K(\theta_K)/S_K(\theta_K)]$, C_K must assume negative values to prevent B_K from incorrectly becoming negative. A similar situation holds also for C_L . Consequently, for low enough energies the C_K and C_L corrections become large and negative.

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Transport and Deformation-Potential Theory for Many-Valley Semiconductors with Anisotropic Scattering

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A transport theory which allows for anisotropy in the scattering processes is developed for semiconductors with multiple nondegenerate band edge points. It is found that the main effects of scattering on the distribution function over each ellipsoidal constant-energy surface can be described by a set of three relaxation times, one for each principal direction; these are the principal components of an energy-dependent relaxation-time tensor. This approximate solution can be used if all scattering processes either conserve energy or randomize velocities. Expressions for mobility, Hall effect, low- and high-field magnetoresistance, piezoresistance, and high-frequency dielectric constant are derived in terms of the relaxation-time tensor. For static-field transport properties the effect of anisotropic scattering is merely to weight each component of the effective-mass tensor, as it appears in the usual theory, with the reciprocal of the corresponding component of the relaxationtime tensor.

1. INTRODUCTION

In the last few years, it has been become clear that most of the well-studied semiconductors have energy band structures greatly different from the simple model

The deformation-potential method of Bardeen and Shockley is generalized to include scattering by transverse as well as longitudinal acoustic modes. This generalized theory is used to calculate the acoustic contributions to the components of the relaxation-time tensor in terms of the effective masses, elastic constants, and a set of deformation-potential constants. For n silicon and n germanium, one of the two deformation-potential constants can be obtained from piezoresistance data. The other one can at present only be roughly estimated, e.g., from the anisotropy of magnetoresistance. Insertion of these constants into the theory yields a value for the acoustic mobility of n germanium which is in reasonable agreement with observation; a more accurate check of the theory may be possible when better input data are available. For n silicon, available data do not suffice for a check of the theory.

which had nearly always been assumed in earlier theoretical work. Whereas this simple model [Fig. 1(a)] assumed a nondegenerate band-edge state with wave vector $\mathbf{K} = 0$ and spherical surfaces of constant energy, many or most actual band structures seem to be either of the "many-valley" type [Fig. 1(b)], with several nondegenerate band-edge points $\mathbf{K}^{(4)}$ and ellipsoidal

¹³ See Table XVI, H. Bethe, *Handbuch der Physik* (Verlag Julius Springer, Berlin, 1933), Vol. 24, Part 1, p. 443.

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¹ For a brief review of some of the evidence, see C. Kittel, Physica 20, 829 (1954).