

by the lower-energy line to n^2 in (33) for the higher energy line is large and negative.

The assumptions which have been made to obtain the theory of the dielectric constant were discussed as they were made. The least satisfying of these is probably the assumption that the general theory is valid for actual crystals which do not fit either extreme exciton model. The theory as constructed in Secs. III through V is a more precise theory than the usual one outlined in Sec. II. The division of the crystal into sub-blocks, the use of semiclassical radiation theory, the assumption that $\epsilon - 1$ is a small quantity, and an appeal to a group velocity were all avoided.

The formulation given of the complex dielectric constant problem makes it possible, in principle, to compute the complex dielectric constant from first principles. Although it is impossible to make really

satisfying calculations on the basis of this theory without much more knowledge of exciton wave functions and the exciton-lattice interaction than is available at present, nevertheless the theory can be of use in providing a framework in which to interpret the optical absorption associated with exciton states.

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Lorentzian Gas and Hot Electrons

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The problem of hot electrons in a nonpolar crystal is reconsidered using the Lorentzian gas model more accurately. Scattering by acoustical phonons alone is considered first. The new results are (1) an asymptotic formula for the moments of the velocity distribution which permits calculation of the deviation from the square root law at high fields, and (2) a recursion system allowing the calculation of any velocity polynomial in terms of the average energy, random velocity, and mobility of the electrons. Scattering by ionized impurities in addition to acoustical phonons is considered next and the distribution function is derived. The proportionality constant relating the change in the low-field mobility to E^2 is shown to be highly sensitive to ionized impurity scattering. Thus, appreciable changes from its value for pure lattice scattering occur for μ_0/μ_I as low as 10^{-3} . (E is the field strength and μ_0 and μ_I are the low-field lattice and impurity mobilities, respectively.) It is pointed out that substantial deviations from results obtained using a Maxwellian distribution do occur.

1. INTRODUCTION

THIS paper concerns the motion of electrons (or holes) in nonpolar semiconductors or insulators in strong electrostatic fields. We consider a crystal with spherical energy bands and at a high enough temperature so that the equipartition law is valid for the acoustical lattice oscillators with which an electron interacts. With these two assumptions, Shockley¹ shows that the scattering cross section² and the average energy losses for an electron interacting with acoustical phonons, remain, to a good approximation, the same if we replace the phonon field by a classical gas of hard spheres of mass³ KT/c^2 (where c is the longitudinal speed of sound and KT is the thermal energy) and of

such a density as to make the mean free path (mfp) the same in both cases. This is the Lorentzian^{4,5} gas model or the gaseous discharge analogy. Indeed, the velocity distribution function is the same in both cases. (See Sec. 2.)

In Sec. 2 we shall give accurate calculations for the physical properties of hot electrons in Shockley's model. In particular, we wish to emphasize deviations from the square root law in the current voltage characteristics at intermediate fields.

In Sec. 3 we shall consider scatterings by ionized impurities, in addition to acoustical phonons, derive the proper distribution function and obtain deviations from Ohm's law at low fields. The results will be compared to those obtained using a Maxwellian distri-

¹ W. Shockley, Bell System Tech. J. **30**, 990 (1951).

² See also F. Seitz, Phys. Rev. **73**, 549 (1948); A. H. Wilson, *The Theory of Metals* (Cambridge University Press, Cambridge, 1953), second edition, Chap. 9.

³ The validity of equipartition implies that KT/c^2 is much greater than the electron effective mass.

⁴ H. A. Lorentz, *Theory of Electrons* (Stechert and Company, New York, 1923), p. 267.

⁵ S. Chapman and T. G. Cowling, *The Mathematical Theory of Nonuniform Gases* (Cambridge University Press, Cambridge, 1953), second edition, p. 187.

bution.⁶ The major difference is that in our calculations ionized impurity scattering is important for rather low densities of ionized impurities. It should be made clear, however, that we assume that electron-phonon collision dominates electron-electron collision, while a Maxwellian distribution represents the other extreme.⁷

2. ACOUSTICAL PHONONS

In the diffusion approximation, the velocity distribution function of electrons, f , is written as $f=f^0+f^1\cos\theta$, where θ is the angle between the directions of the electric field \mathbf{E} and the electron velocity \mathbf{c}_1 . The functions f^0 and f^1 satisfy the Lorentzian gas equations:⁸

$$f^1 = -(qEl/m_1c_1)\partial f^0/\partial c_1, \tag{2.1}$$

$$\frac{qE}{3m_1c_1^2} \frac{\partial}{\partial c_1}(c_1^2 f^1) = \frac{m_1}{m_2c_1^2} \frac{\partial}{\partial c_1} \left\{ \frac{c_1^4}{l} f^0 + \frac{KT}{m_1l} \frac{\partial f^0}{\partial c_1} \right\}, \tag{2.2}$$

where q , l , and m_1 are the electron charge, mean free path, and effective mass, respectively, and $m_2=KT/c^2$. Since l is energy independent, the above equations give

$$f^0 = e^{-x}(1+x/y)^y/f(y, \frac{1}{2}), \tag{2.3}$$

where $x=m_1c_1^2/2KT$, $y=3\pi(\mu_0E/4c)^2$, $\mu_0=\frac{4}{3}ql \times (2\pi m_1KT)^{-\frac{1}{2}}$, the zero-field mobility, and

$$f(y,r) = \int_0^\infty e^{-x}(1+x/y)^y x^r dx. \tag{2.4}$$

Thus, f^0 is normalized to unity.

To evaluate the average of any velocity polynomial we need to know $f(y,r)$ for integral and half-integral values of r . A partial integration of (2.4) gives the recursion system,

$$f(y, r+1) = (r+1)f(y,r) + ryf(y, r-1) + y\delta_{r0}; \tag{2.5}$$

$r \geq 0.$

It is clear from (2.5) that a calculation of $f(y,r)$ for $r=0, \frac{1}{2}, \frac{3}{2}$ is sufficient to generate other integral or half-integral moments. These basic moments have been calculated and used in calculating the mobility, average energy, and random velocity given by μ , ϵ , v , respec-

⁶ M. S. Sodha, Phys. Rev. 107, 1266 (1957).

⁷ See H. Frohlich and B. V. Paranjape, Proc. Phys. Soc. (London) B69, 21 (1956).

⁸ See Chapman and Cowling, reference 4, p. 346. These classical equations can be obtained *directly* by expanding the collision term in a Taylor's series in terms of the energy transfer or change in the velocity magnitude; I. Adawi, Bull. Am. Phys. Soc. Ser. II, 3, 13 (1958). The transport equation for the quantum-mechanical problem of electrons and acoustical phonons can be treated similarly. A Taylor's expansion in terms of the energy transfer is possible as has been done by J. Yamashita and M. Watanabe, Progr. Theoret. Phys. (Japan) 12, 443 (1954); or in terms of change in the electron wave number k , either *directly*, or *indirectly* by applying the method of Chapman and Cowling, and equations identical to (2.1) and (2.2) are obtained [I. Adawi (unpublished)].

tively. Thus

$$\begin{aligned} \mu/\mu_0 &= \frac{1}{2}\pi^{\frac{1}{2}}f(y,0)/f(y,\frac{1}{2}), \\ v/v_0 &= \frac{1}{2}\pi^{\frac{1}{2}}f(y,1)/f(y,\frac{1}{2}), \\ v_0 &= (8KT/\pi m_1)^{\frac{1}{2}}, \\ \epsilon/\epsilon_0 &= \frac{2}{3}f(y,\frac{3}{2})/f(y,\frac{1}{2}), \\ \epsilon_0 &= \frac{3}{2}KT. \end{aligned} \tag{2.6}$$

For $y \ll 1$, $f(y,r)$ is approximated by its tangent at the origin which is equivalent to the Davydov⁹ approximation, $f^0 \propto e^{-x}xy$, and

$$\begin{aligned} \mu/\mu_0 &\approx 1 - 2(1 - \ln 2)y, \\ v/v_0 &\approx 1 + (2 \ln 2 - 1)y, \\ \epsilon/\epsilon_0 &\approx 1 + \frac{2}{3}y. \end{aligned} \tag{2.7}$$

For $y \gg 1$, an asymptotic expansion gives¹⁰

$$\begin{aligned} f(y,r) &\sim 2^{\frac{1}{2}(r-1)}y^{\frac{1}{2}(r+1)}\Gamma[\frac{1}{2}(r+1)]F(r), \\ F(r) &= 1 + \frac{2}{3}(2/y)^{\frac{1}{2}}\Gamma[\frac{1}{2}r+2]/\Gamma[\frac{1}{2}(r+1)] \\ &\quad + (1/18)(r+\frac{1}{2})(r+1)(r+3)y^{-1}, \end{aligned} \tag{2.8}$$

and

$$\begin{aligned} \mu/\mu_0 &\sim 1.08y^{-\frac{1}{2}}F(0)/F(\frac{1}{2}), \\ v/v_0 &\sim 0.86y^{\frac{1}{2}}F(1)/F(\frac{1}{2}), \\ \epsilon/\epsilon_0 &\sim 0.70y^{\frac{1}{2}}F(\frac{3}{2})/F(\frac{1}{2}), \\ F(0) &= 1 + 0.53y^{-\frac{1}{2}} + 0.083y^{-1}, \\ F(\frac{1}{2}) &= 1 + 0.87y^{-\frac{1}{2}} + 0.29y^{-1}, \\ F(1) &= 1 + 1.25y^{-\frac{1}{2}} + 0.67y^{-1}, \\ F(\frac{3}{2}) &= 1 + 1.67y^{-\frac{1}{2}} + 1.25y^{-1}. \end{aligned} \tag{2.9}$$

The set of equations (2.9) give the deviations from the well-known simple laws, $\mu \propto E^{-\frac{1}{2}}$, $v \propto E^{\frac{1}{2}}$, and $\epsilon \propto E$. For $y=100$ these deviations are about 4% in μ and v but about 8% in ϵ . The results of the calculations are presented graphically in Figs. 1-3.

3. IONIZED IMPURITIES

We wish now to include impurity scattering in addition to lattice scattering. Consider fixed and

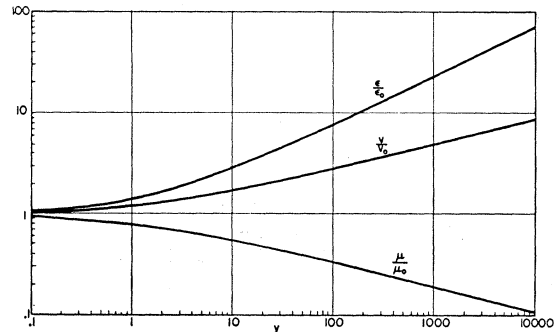


FIG. 1. Reduced mobility, random velocity, and energy as a function of the reduced field parameter y .

⁹ B. Davydov, Physik. Z. Sowjetunion 8, 59 (1935).
¹⁰ In the Druyvesteyn approximation, $f^0 \sim \exp(-x^2/2y)$, $F(r)=1$.

randomly distributed centers of density N_i per unit volume and differential cross section $\sigma_i(\theta, c_1)$, where the index i runs over the different types of impurities, such as ionized, neutral, etc. Such a scattering will not involve any energy loss (at least not within our approximations) and consequently (2.2) will remain unimpaired. The only change is that in (2.1) l will be replaced by an effective mean free path, \bar{l} given by

$$\bar{l} = l\lambda / (l + \lambda),$$

$$\lambda^{-1} = \sum_i 2\pi N_i \int \sigma_i(1 - \cos\theta) \sin\theta d\theta. \quad (3.1)$$

The resulting f^0 will be given by:

$$f^0 = \text{const} \exp \left\{ - \int^x dx \left[1 + \frac{y}{x} \frac{\lambda}{l + \lambda} \right]^{-1} \right\}. \quad (3.2)$$

For ionized impurities, λ is proportional to the square of the energy (aside from a logarithmic term which we shall treat as a constant¹¹) and can be related to the lattice vibrations mean free path, l , through the equation,

$$\lambda = lx^2\alpha^{-2}, \quad \alpha^2 = 6\mu_0/\mu_I, \quad (3.3)$$

where μ_0 and μ_I are the zero-field mobilities of the lattice and ionized impurities, respectively. Using (3.3) in (3.2), we have

$$f^0 \propto \exp \left\{ - \int^x dx \left[1 + yx/(x^2 + \alpha^2) \right]^{-1} \right\}$$

$$= e^{-x} (x^2 + xy + \alpha^2)^{1/2} \exp \left\{ - \frac{1}{2} y^2 \int^x dx (x^2 + xy + \alpha^2)^{-1} \right\};$$

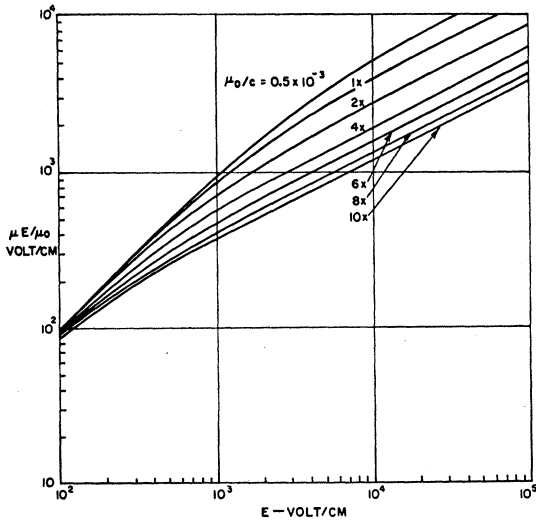


FIG. 2. Drift velocity/ μ_0 vs field strength, for values of μ_0/c ranging from 0.5×10^{-3} to 10×10^{-3} .

¹¹ E. Conwell and V. F. Weisskopf, Phys. Rev. **77**, 388 (1950), see also, for example, P. P. Debye and E. M. Conwell, Phys. Rev. **93**, 693 (1954).

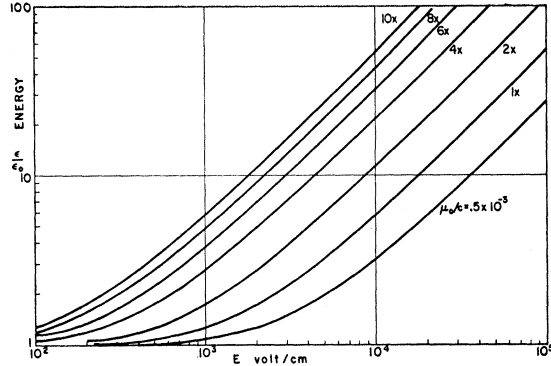


FIG. 3. Electron energy vs field strength, for values of μ_0/c ranging from 0.5×10^{-3} to 10×10^{-3} .

therefore, in general,

$$f^0 \propto e^{-x} (1 + x^2\alpha^{-2})^{1/2} y, \quad y \ll 2\alpha$$

$$\sim e^{-x} (1 + x/y)^y, \quad y \gg 2\alpha. \quad (3.4)$$

Replacing l by \bar{l} in (2.1), we obtain that the combined mobility $\bar{\mu}$ is given by

$$\bar{\mu} = (1/2)\pi^{1/2}\mu_0 \langle x^{-1/2} d/dx [x - \alpha^2 x^2 (x^2 + \alpha^2)^{-1}] \rangle_{f^0}, \quad (3.5)$$

where the average is taken with respect to f^0 normalized to unity. From (3.4) and (3.5) we have for small fields, $y \ll 1$,

$$\bar{\mu}/\mu_0 \approx 1 + \beta y,$$

$$\bar{\mu}_0 = \bar{\mu}(y=0) = (1 - \alpha^2 S_1)\mu_0,$$

$$\beta = [S_1 - (1/8)\alpha^2 L_2^0 + (1/2)\alpha^2 (S_0 - S_1)] / (1 - \alpha^2 S_1) - \pi^{-1/2} L_1^{1/2}, \quad (3.6)$$

where the functions S and L are defined by

$$S_n = \int_0^\infty x^n e^{-x} (\alpha^2 + x^2)^{-1} dx, \quad (3.7)$$

$$L_m^n = \int_0^\infty x^n e^{-x} [\ln(1 + \alpha^{-2} x^2)]^m dx.$$

The integrals S_0 and S_1 are well known,¹² while L_2^0 and $L_1^{1/2}$ have to be evaluated numerically. For large α ($\alpha \sim 20$) we can develop the asymptotic expansion,

$$\beta \sim (33/8)\alpha^{-2} (1 - 81.875\alpha^{-2}) / (1 - 20\alpha^{-2}). \quad (3.8)$$

It is found that $\beta < 0$ for $0 \leq \alpha < 1.02$ and $\beta > 0$ for $\alpha > 1.02$. We can say that in the former range of α lattice scattering is dominant and in the latter range ionized impurity scattering dominates. β assumes a maximum value of 0.072 at $\alpha \approx 2.8$. Figure 4 shows β versus α .

In Table I, our values of the parameter β are compared with those obtained by Sodha⁵ using a Max-

¹² The values of S_0 and S_1 tabulated by R. B. Dingle *et al.*, Appl. Sci. Research **B6**, 155 (1956), can be used for $\alpha < 10$. More accuracy is needed for larger α to obtain β to two significant figures.

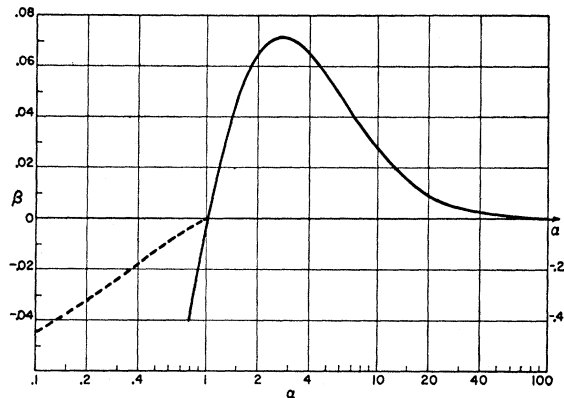


FIG. 4. The coefficient β vs α . The ordinate scale on the right is to be taken with the dotted curve.

wellian distribution for f^0 instead of that given by Eq. (3.4). Sodha's values are denoted by β' , where $\beta' = \frac{1}{2} f_1(a_1)$ in Sodha's Eq. (15.1). From this table we see that both β and β' change sign when α is slightly greater than 1, and assume a maximum for about the same value of α ($\alpha \approx 2.8$) although the maximum value of β' is about 15% larger than that of β . For $\alpha \gg 1$, we have $\beta' \sim 4.5\alpha^{-2}$ which is about 9% higher than the leading term of Eq. (3.8). For $\alpha < 1$, β and β' differ in general by a factor of two to three.

A major difference between our results and those based on a Maxwellian distribution lies in the sensitivity of the parameter β to ionized impurity scattering. From the first two rows of Table I, we observe that for pure lattice scattering ($\alpha=0$), $\beta = -0.61$, and that for a slight ionized impurity scattering corresponding to $\alpha=0.1$ or ($\mu_0/\mu_I = 1/600$), $\beta = -0.44$ which is a substantial change of about 28%. The corresponding change in β' is less than 10%. At the same time $\bar{\mu}_0$, which is Ohm's law mobility, changes only by 2%. We recall from Eqs. (3.3) and (3.6) that α^2 measures the ratio of scattering by ionized impurities to that of lattice vibrations and β measures deviations from Ohm's law, or the field-dependent part in the mobility, at small fields. Thus a change in Ohm's law mobility of 2% due to ionized impurity scattering is accompanied by a change of 28% in the field-dependent part of the mobility at low fields, if electron-electron collision can be ignored. In case that electron-electron interaction is not sufficiently strong to impose a Maxwellian

distribution, the actual value of β is expected to lie between the extreme values of β and β' given in Table I.

TABLE I. A comparison of β and β' for different α 's.

α	β	β'
0	-0.61	-0.25
0.1	-0.44	-0.23
1	-0.003	-0.01
2	+0.065	+0.077
3	0.072	0.083
4	0.065	0.078
8	0.036	0.059
10	0.027	0.043
15	0.015	0.022
20	0.009	0.010

Note added in proof.—We have recently developed a variational method, particularly suited for calculating β under general scattering mechanisms. If we select the

representation, $f^0 \propto e^{-x}(1 + \sum_{r=1}^n b_r x^r)$, then the coefficients

b_r can be determined by variational methods. If we take $n=1$, then $b_1 = (1/2)S_3 y$, and this distribution is identical to the Maxwellian distribution to order y (or E^2) and reproduces Sodha's results. If we take two terms, $n=2$, and let $\alpha \gg 1$; then to order α^{-2} , $b_1=0$ and $b_2 = (1/2)\alpha^{-2}y$, and the distribution is identical to that obtained from (3.4) by writing $(1 + \alpha^{-2}x^2)^{(1/2)y} \sim 1 + (1/2)y\alpha^{-2}x^2$. Indeed, this distribution gives the same leading term as the asymptotic formula (3.8). For small α , a large number of terms is needed. Using three terms, we obtain for $\alpha=0$, $\beta = -0.41$ as compared to -0.61 . A function involving $\ln x$, or $\ln x$ itself which is exact, should be added to the series as a trial solution. Thus, for example, if $f^0 \propto e^{-x}(1 + by \int_x^\infty dt e^{-t}/t)$, then $b = -\frac{3}{2}$ and $\beta = -0.52$ for $\alpha=0$.

We have proved in general that to order E^2 , a Maxwellian distribution is a solution in a variational sense, (although it could be a poor one in certain instances as has been illustrated here), provided the collision operator is linear.

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