Maximum Anisotropy Approximation for Calculating Electron Distributions; Application to High Field Transport in Semiconductors

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The conventional spherical harmonics expansion of the electron distribution function has been useful in obtaining solutions of the Boltzmann equation under circumstances in which the distribution function is fairly isotropic. This same expansion is here used under conditions in which the distribution is distorted by the presence of a large number of electrons streaming along the direction of the electric field. The innovation is a change in the truncation procedure used to obtain a closed system of equations from the infinite hierarchy of equations which result when the spherical harmonics expansion is inserted into the Boltzmann equation. The new method is applied to the calculation of the electron distribution in a semiconductor in the presence of a strong electric field. The resulting analytic distribution functions and ionization rates are compared with numerical computations in which the Boltzmann equation was solved with no approximations about the angular dependence. Agreement is of the order of 10-15% over a range of parameters for which the ionization rates vary through three and one half decades.

I. INTRODUCTION

IN situations in which electron-electron interactions play a negligible role, the velocity distribution of electrons under the influence of a dc electric field may become highly peaked along the field direction. For example, the observed field dependence of the Townsend alpha coefficient which is roughly $\exp(-b/\mathcal{E})^{1,2}$ \mathcal{E} being the strength of the field, has been interpreted as resulting from electrons whose motion is fully parallel to the field.3 Calculations of the angular distribution of electrons in the avalanche breakdown of hydrogen also reveal a marked elongation.4 It would clearly be useful for the interpretation of high-field transport experiments to have a simple analytic method of calculating the distribution function under circumstances in which this streaming along the field direction seriously distorts the distribution. The present work is an account of such a method.

The approximation to be described is nothing more than a new truncation scheme for breaking off the infinite series of equations which result when a spherical harmonics expansion of the distribution function is inserted into the Boltzmann equation. In spite of the extreme simplicity of the idea (or perhaps in addition to it), this new method has several features to recommend it. Firstly, it is as tractable as the more common P_N or generalized diffusion theory approximation⁵; it leads to equations of nearly the same form as those of the P_N method which can be solved with the moderate amount of effort normally expended on obtaining a P_N solution. Secondly, it provides a sort of upper bound to

those transport parameters for which the P_N method provides the lower bound and vice versa. Thirdly, although it is designed to be accurate for a sharply peaked distribution, it yields exactly the results of the P_N method in that isotropic limit for which the P_N approximation is known to be valid. Finally, it is much easier to use than is the integral equation approach in which no angular approximations are made.6 The distributions calculated by this approximation will be shown to agree well with those calculated by the more cumbersome exact method.

In the second section of this paper, the truncation scheme will be described in general terms. The specialization to the description of the spatially-independent high-field distribution function in semiconductors will be found in Sec. III (energy below ionization threshold) and Sec. IV (energy above ionization threshold). From these two sections emerges an explicit expression for the distribution function which, in Sec. V, is exhibited and used to compute the Townsend alpha coefficient.

II. THE NEW TRUNCATION

Under the influence of an electric field in the z direction, the distribution function $f(\mathbf{r},\mathbf{p})$ for electrons in an infinite, isotropic, uniform medium can depend only on z the coordinate in the field direction, c the magnitude of the momentum, and μ the cosine of the angle between the momentum and the field.7 Hence, the distribution function may be expanded as a series of Legendre polynomials

$$f(z,c,\mu) = \sum_{l=0}^{\infty} n_l(z,c) P_l(\mu),$$
 (2.1)

and the coefficients $n_l(z,c)$ may be determined by inserting this expansion in the Boltzmann equation governing electrons in the presence of a uniform dc

⁶ G. A. Baraff, Phys. Rev. 128, 2307 (1962).

⁷ It is assumed that the velocity V is parallel to the momentum

¹ C. A. Lee et al. (to be published).

A. G. Chynoweth, J. Appl. Phys. 31, 1161 (1960).
 W. Shockley, Solid State Electron. 2, 35 (1961).
 G. A. Baraff and S. J. Buchsbaum, Phys. Rev. 130, 1007

⁽¹⁹⁶³⁾ ⁵ This is the name given, in neutron transport theory, to the method of approximating the distribution function by using N spherical harmonics. The lowest order, or P_1 method, leads exactly to the ordinary equation of diffusion theory. See, for example R. L. Murray, in *Nuclear Reactor Physics* (Prentice Hall, Inc., Englewood Cliffs, New Jersey, 1957).

electric field:

$$\left(V_z \frac{\partial}{\partial z} + e \mathcal{E} \frac{\partial}{\partial p_z} + \frac{1}{\tau}\right) f = \left(\frac{\partial f}{\partial t}\right)_{\text{scatter in}}.$$
(2.2)

The τ on the left of Eq. (2.2) is the momentum-dependent mean free time for collisions of all types and therefore the term f/τ represents the rate at which electrons are scattered out of the element at z, p. The term on the right represents scatter *into* the momentum range at p from other momenta. It is not necessary to specify it in detail here beyond asserting that it too can be expanded as a Legendre series which will in general contain but a few terms

$$\left(\frac{\partial f}{\partial t}\right)_{\text{scatter in}} = \sum_{l=0} S_l(z,c) P_l(\mu). \tag{2.3}$$

Before inserting the series expansions into the Boltzmann equation, one may introduce polar coordinates

$$c = (p_x^2 + p_y^2 + p_z^2)^{1/2}$$
 (2.4a)

$$\mu = p_z/c \tag{2.4b}$$

and the mass, m

$$\mathbf{V} = \mathbf{p}/m \,, \tag{2.4c}$$

so as to be able to write the collisionless terms in the Boltzmann equation as

$$V_{z} \frac{\partial}{\partial z} + e \mathcal{E} \frac{\partial}{\partial p_{z}} = \frac{c}{m} \frac{\partial}{\partial z} + e \mathcal{E} \left(\mu \frac{\partial}{\partial c} + \frac{(1 - \mu^{2})}{c} \frac{\partial}{\partial \mu} \right). \quad (2.5)$$

The effect of these terms on the Legendre polynomials is given by⁸

$$\mu P_l(\mu) = (2l+1)^{-1} [(l+1)P_{l+1} + lP_{l-1}], \quad (2.6a)$$

$$(1-\mu^2)\frac{\partial}{\partial \mu}P_l(\mu) = (2l+1)^{-1}l(l+1)[P_{l-1}-P_{l+1}]. \quad (2.6b)$$

When the two Legendre series Eqs. (2.1) and (2.3) are substituted into the Boltzmann equation, use of Eqs. (2.5) and (2.6) allows the coefficient of each Legendre polynomial to be identified. Since the various polynomials are mutually orthogonal, the coefficient of each must be separately annulled. This results in an infinite set of equations, the first few of which are

$$e\mathcal{E}_{3}^{1}\left[n_{1}'+\frac{2}{c}n_{1}\right]+\frac{n_{0}}{\tau}=S_{0},$$

$$e\mathcal{E}_{5}^{2}\left[n_{2}'+\frac{3}{c}n_{2}\right]+e\mathcal{E}(1/1)\left[n_{0}'-\frac{0}{c}n_{0}\right]+\frac{n_{1}}{\tau}=S_{1}, \quad (2.7)$$

$$e\mathcal{E}(3/7)\left[n_{3}'+\frac{4}{c}n_{3}\right]+e\mathcal{E}_{3}^{2}\left[n_{1}'-\frac{1}{c}n_{1}\right]+\frac{n_{2}}{\tau}=S_{2},$$

with the prime denoting the differentiation

$$n_{l}' \equiv \left(\frac{\partial}{\partial c} + \frac{c}{me \, \mathcal{E}} \frac{\partial}{\partial z}\right) n_{l}(z,c) \,. \tag{2.8}$$

Any finite number N of these equations contain in general (N+1) unknown coefficients. Since the information of physical interest is usually contained in the expansion coefficients of low l, the problem is to truncate the set (2.7) so that the first N equations contain only the first N unknown coefficients.

The generalized diffusion theory approximation follows from the assumption that the distribution (2.1) is nearly isotropic. In that case, the coefficients will decrease rapidly with increasing l. The natural truncation is then to set n_N equal to zero, which allows the first N equations to be solved. The maximum anisotropy approximation, on the other hand, follows from the assumption that the distribution is highly elongated, so that the convergence of the series is extremely slow. Perhaps the slowest convergence of all would be obtained when the electrons were all traveling in the direction of acceleration, i.e., if the distribution function were zero unless $\mu=1$. Such a distribution would contain the Dirac delta function for its angular dependence, and would be written

$$f(z,c,\mu) = g(z,c)\delta(1-\mu)$$
. (2.9)

Since the expansion coefficients of (2.1) can be determined from a *known* distribution f by means of

$$n_l(z,c) = \frac{2l+1}{2} \int_{-1}^1 f(z,c,\mu) P_l(\mu) d\mu \qquad (2.10)$$

a distribution of the form (2.9) would lead to

$$n_l(z,c) = [(2l+1)/(2l-1)]n_{l-1}(z,c)$$
.

It would seem likely that this behavior at high values of l would be the slowest convergence to be expected for any physical distribution. It is thus as reasonable to truncate the Eqs. (2.7) by setting

$$n_N(z,c) = [(2N+1)/(2N-1)]n_{N-1}(z,c)$$
 (2.11)

in situations where great elongation is expected as it is to truncate by setting n_N equal to zero in situations where near isotropy is expected. The equations truncated in this way would lead to the exact distribution function only if the exact distribution were really of the form (2.9). This scheme would seem at first to become less valid as the distribution becomes more isotropic. In the limit of near isotropy, however, the last retained expansion coefficient is so small that replacing it by something of order unity times itself makes negligible

⁸ H. Margenau and G. M. Murphy, *The Mathematics of Physics and Chemistry* (D. Van Nostrand Company, Inc., Princeton, New Jersey, 1943).

⁹ See also P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Chap. 12.

¹⁰ The coupling to the higher n_l arises almost invariably through the first term on the left of each of the Eqs. (2.7). The structure of the scattering terms S_l is usually such that S_N involves only those n_l for which $l \le N$. These cause no coupling to higher l coefficients.

change in the equations. This means that the truncation can lead to exact results again in the limit of complete isotropy.

III. DISTRIBUTION BELOW THRESHOLD

In this section and the next the maximum anisotropy assumption is applied in a simple way to the calculation of the spatially uniform z-independent high-field distribution for electrons (or holes) in a semiconductor. Applying the truncation (2.11) to Eqs. (2.7) with N=2 makes the third and all higher equations irrelevant and converts the first two to the following pair of coupled equations:

$$e\mathcal{S}_{3}^{1}\left[\frac{dn_{1}}{dc} + \frac{2}{c}n_{1}\right] + \frac{n_{0}}{\tau} = S_{0},$$

$$e\mathcal{S}_{3}^{2}\left[\frac{dn_{1}}{dc} + \frac{3}{c}n_{1}\right] + e\mathcal{S}_{dc} + \frac{n_{1}}{\tau} = S_{1}.$$
(3.1)

It is necessary now to specify τ and the S_l terms. Recent avalanche breakdown experiments of Lee, Logan, Batdorf¹ et al. are in reasonable agreement with calculations based on the following assumptions:

There are two processes which contribute to the scattering represented by τ , namely, optical-phonon emission and ionization. There is a threshold energy E_i below which no ionization occurs and above which the ionization mean free path l_i is constant. Optical phonon emission alone would yield a constant mean free path λ .

Emission of an optical phonon is an isotropic scattering event which reduces the energy of the electron by amount E_R , the (assumed constant) optical-phonon energy. Ionization is an event in which the energy of the electron is reduced to zero. The reader is referred to Wolff's paper on electron multiplication¹¹ for a clear discussion of why these assumptions are reasonable idealizations for high-field semiconductor transport; the agreement between the avalanche breakdown measurements and calculation provide tentative confirmation that the assumptions may have some validity for silicon. In mathematical terms, these assumptions take the form¹¹

$$\frac{1}{\tau} = \frac{c}{m} \left(\frac{1}{\lambda} + \frac{1}{l_i} \right) \tag{3.2a}$$

$$S_0(c) = (2/c\lambda)(E + E_R)n_0(c')$$
 (3.2b)

$$S_1(c) = 0$$
 (3.2c)

$$c' = \lceil 2m(E + E_R) \rceil^{1/2},$$
 (3.2d)

where l_i is to be regarded as infinite for energies below the ionization threshold and the energy E is $c^2/2m$. It is convenient to use E rather than c as the independent variable and to define

$$m_0(E) = En_0(c) \tag{3.3a}$$

$$m_1(E) = En_1(c) \tag{3.3b}$$

$$Q = e \mathcal{E} l_i r \tag{3.4a}$$

$$r = \lambda/(\lambda + l_i)$$
. (3.4b)

The term $m_0(E+E_R)$ which then appears in $S_0(c)$ may be replaced by the first two terms of its Taylor series expansion with the result that Eqs. (3.1) take the form

$$\frac{Q}{3}\frac{dm_1}{dE} + rm_0(E) - (1 - r)E_R \frac{dm_0}{dE} = 0$$
 (3.5a)

$$\frac{2Q}{3}\frac{dm_1}{dE} + \left(1 + \frac{Q}{3E}\right)m_1 + QE\frac{dn_0}{dE} = 0.$$
 (3.5b)

Consider the energy range below threshold. In this range, r=0, $Q=e\mathcal{E}\lambda$ and Eq. (3.5a) yields

$$m_0 = (Q/3E_R)m_1 + A$$
, (3.6)

where A is a constant of integration. Using this m_0 , Eq. (3.5b) becomes

$$dm_1/dE + (b+a/E)m_1 = QAb/E$$
 (3.7)

with

$$a = \frac{1 - Q/E_R}{2 + Q/E_R}; \quad \frac{1}{b} = \frac{2Q}{3} + \frac{Q^2}{3E_R}.$$
 (3.8)

The solution to this equation for m_1 is

$$m_1(E) = (QAb/a)\{1 + \Re(E) - (E/E_i)^{-a} \exp[b(E_i - E)]\} + [m_1(E_i)](E/E_i)^{-a} \exp[b(E_i - E)], \quad (3.9)$$

where

$$\mathcal{K}(E) = bE^{-a}e^{-bE}\int_{E}^{E_{i}} t^{a}e^{bt}dt. \tag{3.10}$$

There are two integration constants, A and $m_1(E_i)$, appearing in Eqs. (3.9) and (3.6). It is convenient to fix them in terms of

$$\alpha \equiv \alpha(E_i) \equiv m_1(E_i)/m_0(E_i) \tag{3.11a}$$

and a normalization condition

$$m_0(E_i) = 1.$$
 (3.11b)

The constant α will depend on the solution in the ionizing region. Evaluating (3.6) at $E=E_i$ gives

$$A = 1 - Q\alpha/3E_R$$
. (3.12)

The explicit solutions for m_0 and m_1 are now contained in Eqs. (3.6), (3.9)–(3.12) and can be written out in full as soon as α is determined.

Although the function $\mathcal{K}(E)$ cannot be simplified further, a power series expansion makes it only slightly more difficult to evaluate than other functions which can be expressed in closed form. The details will be found in Appendix A.

¹¹ P. A. Wolff, Phys. Rev. 95, 1415 (1954).

It is interesting to consider the form of m_0 in the limit $Q=E_R$. From the definition of Q, it is apparent that an electron starting from rest will acquire an energy equal to Q at about the time of its first collision. At this collision, it will lose an amount of energy E_R . Hence, if $Q=E_R$, the average electron loses all its energy on its first collision and only those electrons which avoid collision can attain an energy greater than E_R . The number which reach energy E is proportional to $\exp(-E/Q)$. These are the electrons considered by Shockley in explaining avalanche breakdown. The function $m_0(E)$ is also proportional to the number of electrons at energy E. We may anticipate the results of the next section and use the evaluation $\alpha=3$ when $Q=E_R$. Referring to (3.8), one finds that a=0, $b=Q^{-1}$ in this limit, so that for $Q = E_R$,

$$m_0(E) = \exp[(E_i - E)/Q].$$

That this agrees exactly with the distribution proposed by Shockley is not surprising: in this limit, the electrons are streaming along the field direction and the maximum anisotropy approximation was devised, after all, with this situation in mind. What is surprising is the behavior of $m_0(E)$ in the limit $Q/E_R\gg 1$. In this high-field limit, the energy loss per collision is so much smaller than the energy gain per collision of electrons traveling along the field direction that most of the electrons will not be traveling along the field, i.e., the collisions will randomize the velocities and the distribution will be nearly isotropic. Under these conditions, the results of Wolff¹¹ should be valid. Referring to Eq. (3.8) again, one finds that in the limit, $Q\gg E_R$, a=-1, $b=3E_R/Q^2\equiv W^{-1}$ so that after making some obvious rearrangements,

$$n_0(E) = A_1 e^{-E/W} + B_1 e^{-E/W} \int_{-\infty}^{E} e^{t/W} \frac{dt}{t},$$
 (3.13)

where A_1 and B_1 are constants which depend on α , i.e., which may be determined by considering the behavior of the solution in the ionizing region. This is *precisely* the solution given by Wolff using the P_1 approximation.

Thus, the maximum anisotropy approximation is able to accurately represent the distribution in the two limiting cases $Q=E_R$ and $Q\gg E_R$. There is a strong possibility that it may not be too much in error for the intermediate cases.

IV. DISTRIBUTION ABOVE THRESHOLD

This section is concerned with the solution in the ionization region $E > E_i$ for which $r \neq 0$. It is useful though to think first about a situation in which $E_i = 0$ and r = 1. The only particles at elevated energies will then be those which have escaped all collisions. Their distribution is

$$m_0(E) = \exp(-E/Q)$$
 (4.1a)

and, for such a distribution,

$$\int_{E}^{\infty} m_0(E') dE' = Q m_0(E). \tag{4.1b}$$

If, for r < 1, the distribution were exponential with decrement lQ instead of Q, then lQ would replace Q in both Eqs. (4.1). If, moreover, the distribution were almost but *not quite* exponential, then the quantity l(E) defined by

$$\int_{E}^{\infty} m_0(E')dE' = Ql(E)m_0(E) \tag{4.2}$$

would be almost but not quite independent of energy.

It is well known in neutron transport that the distribution in a partially absorbing medium is extremely similar to the distribution in a fully absorbing medium unless the probability that a particle be absorbed on a given collision is very much less than unity. By analogy, the distribution in the electron transport problem for r < 1 should be close to the r = 1 distribution unless r is very small. But at the limit of r = 0, the situation reduces to that of the last section for which the solution

$$m_0(E) = E^{-a}e^{-bE}, -1 < a < \frac{1}{2}$$

has been given. This solution deviates only weakly, for $E > E_i$, from a pure exponential. Hence, for r = 0 we expect l to differ only weakly from a constant value b, while for r much greater than zero we expect l = 1, again independent of energy. That is, the l(E) defined by (4.2) is likely to be a weak function of energy for all values of r. One may integrate Eq. (3.5a) from E to infinity with the result

$$m_1(E) = \alpha(E)m_0(E) \tag{4.3}$$

$$\alpha(E) = 3(1-r)E_R/O + 3rl(E)$$
. (4.4)

If l(E) is nearly independent of energy, then $\alpha(E)$ will be nearly constant. An exact equation governing $\alpha(E)$ may be used to determine that constant.

Before constructing this equation, however, it is desirable to replace the phonon energy E_R appearing in Eqs. (3.5a) and (4.4) by E_R^* , an effective phonon energy which reduces to E_R in the absence of absorption, i.e., at r=0. The desirability of this replacement arises because the approximation

$$m_0(E+E_R) \cong m_0(E) + E_R(dm_0/dE)$$
,

which converts the difference equation (3.1) into the differential equation (3.5) is not as accurate for this purpose as is the replacement

$$m_0(E+E_R) \cong m_0(E) + E_R^*(dm_0/dE)$$
 (4.5a)

$$E_R^* = \{ [(1-r)^{-1} - 1] / \ln(1-r)^{-1} \} E_R.$$
 (4.5b)

¹² K. M. Case, F. de Hoffman, and G. Placzek, *Introduction to the Theory of Neutron Diffusion* (U. S. Government Printing Office, Washington, D. C., 1953).

The derivation of this result is completely elementary and may be found in Appendix B.

The equation governing $\alpha(E)$ is constructed using (4.3) and (3.5b) as follows: From Eqs. (4.3) and (3.3) one constructs

$$dn_0/dE = d(E^{-1}\alpha^{-1}m_1)/dE$$
,

which is substituted into Eq. (3.5b) to yield

$$dm_1/dE + m_1(E)f(E) = 0$$
 (4.6)

$$f(E) = \left[\frac{1}{Q} + \left(\frac{1}{3} - \frac{1}{\alpha}\right)\frac{1}{E} + \frac{d\alpha^{-1}}{dE}\right] / \left(\frac{2}{3} + \frac{1}{\alpha}\right). \quad (4.7)$$

From Eq. (4.6) one obtains

$$m_1(E) = m_1(E_i) \exp \left[-\int_{E_i}^{E} f(E'') dE'' \right]$$
 (4.8)

or, using (4.3) and (3.11)

$$m_0(E) = \left[\alpha(E_i)/\alpha(E)\right] \exp\left[-\int_{E_i}^E f(E^{\prime\prime})dE^{\prime\prime}\right].$$
 (4.9)

From this form for m_0 , the expression l(E) may be constructed by the integration indicated in Eq. (4.2) and the expression so obtained may be used in Eq. (4.4) to give

$$\alpha(E) = \frac{3}{Q} \left\{ (1 - r)E_R^* + r \int_E^\infty \frac{\alpha(E)}{\alpha(E')} dE' \right.$$

$$\times \exp \left[- \int_E^{E'} f(E'') dE'' \right] \right\}. \quad (4.10)$$

This is the exact equation governing $\alpha(E)$. Its solution in those limiting cases for which α is independent of E are

$$a:$$
 If $r=0$, then $\alpha=3E_R/Q$,

b: If
$$r=1$$
, then $\alpha=3$,

c: If
$$Q = E_R^*$$
, then $\alpha = 3$,

as may be easily verified. Used in Eqs. (4.7) and (4.9), these solutions yield

a:
$$m_0 = (E/E_i)^{-a} \exp[-b(E-E_i)]$$

b, c: $m_0 = \exp[-(E-E_i)/Q]$.

The first of these is the part of the pure scattering solution which vanishes at infinity, and the second is the Shockley spike.

This is as far as one can go with no approximations. Since, however, the energy dependence of α is expected to be weak, one may consider an iterative solution of Eq. (4.10) starting with a zeroth order iterate $\alpha(E) = \alpha$, a constant. Inserting this approximation on the right

of Eqs. (4.7) and (4.10) gives

$$\alpha(E) = \frac{3}{Q} \left[(1 - r) E_R^* \right]$$

$$+r\int_{E}^{\infty} \left(\frac{E'}{E}\right)^{-a^*} \exp[-b^*(E'-E)]dE'$$
, (4.11)

with

$$a^* = (1 - 3/\alpha)/(2 + 3/\alpha)$$
 (4.12a)

$$1/b^* = 2Q/3 + Q/\alpha$$
. (4.12b)

The replacement E' = E + t converts (4.11) to

$$\alpha(E) = \frac{3}{Q} \left[(1 - r)E_R^* + r \int_0^\infty (1 + t/E)^{-a^*} e^{-b^*t} dt \right]. \quad (4.13)$$

In this form it is apparent that $\alpha(E)$ will be independent of E only if the exponential cuts off the integrand before the E dependence of the other factor of the integrand becomes appreciable. Since the exponential acts, in effect, to limit t to values of less than about b^{-1} , the condition that α be constant is that

$$(1+1/Eb^*)^{-a^*} \approx 1 - (a^*/Eb^*) \approx 1$$
. (4.14)

In terms of the definitions (4.11), this criterion is

$$\left|\frac{1}{3} - 1/\alpha\right| \ll E/Q. \tag{4.15}$$

Since α is positive, this will certainly be satisfied whenever $\alpha \gg Q/E$.

Assuming, for the moment, that (4.15) is valid, then (4.14) may be used in the integrand of (4.13), giving

$$\alpha = 3(1-r)E_R^* + 3r/(Qb^*)$$
 (4.16)

which, via Eq. (4.12b) is a quadratic equation for α . The solution is

$$\alpha = r + 3(1 - r)E_R^*/2Q + \{3r + \lceil r + 3(1 - r)E_R^*/2Q \rceil^2\}^{1/2}. \quad (4.17)$$

From it, one may check that the inequality (4.15) is satisfied for $E > E_i$ in any case of interest. Having determined α , the quantity f in (4.7) is determined and $m_0(E)$ in (4.9) may be evaluated as

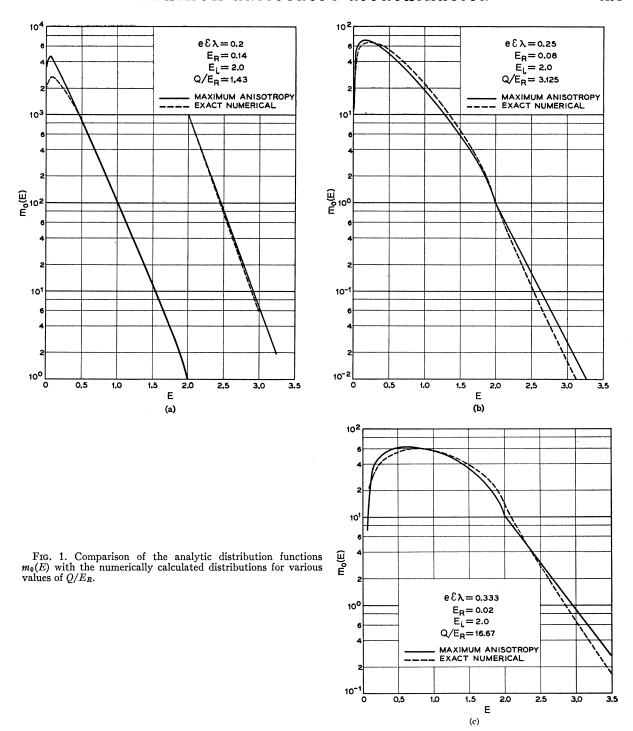
$$m_0(E) = (E/E_i)^{-a^*} \exp[-b^*(E-E_i)].$$
 (4.18)

Also, the constant value of α is to be used in Eq. (3.12) to complete the solution in the region below threshold.

Note that the Q in the region above threshold energy will be different from Q in the region below threshold since the total mean free path above threshold is, in general, shorter than that below.

V. COMPARISON WITH NUMERICAL SOLUTION

To obtain the distribution functions $m_0(E)$ and $m_1(E)$, it is necessary only to compute; the functions and constants on which they depend have all been given in explicit form. In Figs. 1(a), (b), and (c), the distri-



bution function $m_0(E)$ has been compared with the collision density, M(E), to which it should be equal, as calculated using the integral equation method. This calculation was made specifically to compare the maximum anisotropy approximation with the exact integral equation calculation. We have let λ , the mean free path for phonon emission, be stepwise constant,

equal to l_i (mean free path for ionization) for energy E above E_i , and equal to one-half l_i for E above E_i . In this way, Q is constant and does not change at threshold energy. This does *not* correspond to the physics, but the integral equation calculation was not feasible for a stepwise constant Q and the comparison had to be made in this way. The values of Q/E_R and

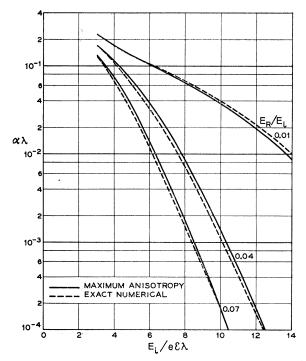


Fig. 2. Comparison of the Townsend alpha coefficient calculated using the analytic distribution functions with the exact numerical calculations.

 E_i/E_R to which these distributions correspond appear on the figures.

It should be apparent from the discussion of Sec. III that the parameter which most fully determines the anisotropy of the distribution is Q/E_R . The three cases selected for comparison with the numerical calculation in Fig. 1 have been chosen to exhibit how the accuracy of the method depends on this parameter.

Perhaps a better over-all comparison between the two methods may be obtained by comparing the Townsend alpha coefficient α_T as calculated by each scheme:

$$\alpha_T = \left[\int d^3 p \ f(\mathbf{p}) / \tau_i(p) \right] / \int d^3 p \ V_z f(\mathbf{p}) \quad (5.1)$$

which, using Eqs. (2.10), (3.2a) and (3.4b) is

$$\alpha_T \lambda = \int_0^\infty r(E) m_0(E) dE / \left[\frac{1}{3} \int_0^\infty m_1(E) dE \right]. \quad (5.2)$$

The comparison between the two methods of computing α_T appears as Fig. 2, in which the "exact numerical result" has been taken from Ref. 6. The over-all agreement of the curves is within 15% over a three and a half decade range of alpha. Neglect of the E_R^* correction, Eq. (4.5), gives much poorer agreement at the large phonon energies.

In conclusion, this paper has presented an approxi-

mation scheme for calculating the classical singleparticle distribution function under conditions where the ordinary P_N approximation fails. The simple model used to describe high field transport in semiconductors leads to an explicit expression for the distribution function which is in extremely close agreement with much more elaborate numerical calculations in which the angular dependence is treated exactly.

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APPENDIX A

We wish to derive the series which may be used to evaluate the function $\mathfrak{X}(E)$

$$\mathcal{K}(E) = bE^{-a}e^{-bE} \int_{R}^{E_i} t^a e^{bt} dt.$$
 (A1)

Let

$$\gamma = bE_i$$
, $A = 1 - E/E_i$, $t = E_i(1 - x)$. (A2)

Then,

$$\mathcal{K}(E) = \gamma e^{\gamma A} (E/E_i)^{-a} \int_0^A (1-x)^a e^{-\gamma x} dx. \quad (A3)$$

Since A < 1, we may expand $(1-x)^a$ as a power series which will converge at all points in the integrand

$$(1-x)^{a} = 1 - ax + [a(a-1)/2!]x^{2} \cdots$$

$$= \sum_{n=1}^{\infty} \frac{x^{n}}{(-a)(1-a)(2-a)\cdots(r-1-a)} \quad (A4)$$

and hence, we may integrate term by term to obtain

$$\mathcal{K} = \gamma e^{\gamma A} (E/E_i)^{-a} \sum_{r=0}^{\infty} (-a)(1-a) \cdots (r-1-a)I_r, \quad (A5)$$

where

$$I_r = \frac{1}{r!} \int_0^A x^r e^{-\gamma x} dx$$

$$= \frac{1}{r!} \left(-\frac{d}{d\gamma} \right)^r \int_0^A e^{-\gamma x} dx$$

$$= \frac{1}{r!} \left(-\frac{d}{d\gamma} \right)^r \left[\frac{1 - e^{-\gamma A}}{\gamma} \right]. \tag{A6}$$

The binomial form for derivatives

$$\bigg(\!-\frac{d}{d\gamma}\!\bigg)^{\!r}\!f(\gamma)g(\gamma)$$

$$=\sum_{p=0}^{r}\frac{r!}{p!(r-p)!}\left[\left(-\frac{d}{d\gamma}\right)^{p}f\right]\left[\left(-\frac{d}{d\gamma}\right)^{r-p}g\right]$$

may be used with

$$f(\gamma) = 1 - e^{-\gamma A}$$
, $g(\gamma) = 1/\gamma$,

so that

$$\left(-\frac{d}{d\gamma}\right)^p f = \delta_{p,0} - A^p e^{-\gamma A}, \quad \left(-\frac{d}{d\gamma}\right)^{r-p} g = \frac{(r-p)!}{\gamma^{r-p+1}}.$$

Hence,

$$I_r = \sum_{p=0}^r \frac{1}{p! \gamma^{r-p+1}} \left[\delta_{p0} - A^p e^{-\gamma A} \right]$$

$$= \frac{1}{\gamma^{r+1}} - \frac{e^{-\gamma A}}{\gamma^{r+1}} \sum_{p=0}^{r} \frac{(\gamma A)^p}{p!}.$$
 (A7)

Note that

$$\sum_{p=0}^{r} \frac{(\gamma A)^p}{p!} = \sum_{p=0}^{\infty} \frac{(\gamma A)^p}{p!} - \sum_{p=r+1}^{\infty} \frac{(\gamma A)^p}{p!}$$
$$= e^{\gamma A} - \sum_{p=r+1}^{\infty} \frac{(\gamma A)^p}{p!}.$$

Hence,

$$I_r = \left(\frac{1}{\gamma^{r+1}}\right) e^{-\gamma A} \sum_{p=r+1}^{\infty} \frac{(\gamma A)^p}{p!}.$$
 (A8)

Insert this into (A5) and reverse the order of summation to obtain

$$\mathcal{K}(E) = (E/E_i)^{-a} \sum_{p=1}^{\infty} \frac{(\gamma A)^p}{p!} \times \sum_{r=0}^{p-1} \frac{(-a)(1-a)(2-a)\cdots(r-1-a)}{\gamma^r}.$$
 (A9)

APPENDIX B

In this Appendix, the effective phonon energy E_R^* which must replace E_R will be calculated by considering Eq. (3.5a) in its unexpanded form

$$(Q/3)(dm_1/dE) = (1-r)m_0(E+E_R) - m_0(E)$$
. (B1)

This equation is the only one in either the P_N approximation or the maximum anisotropy approximation which involves E_R in any way when the scatter is isotropic, so the following derivation applies equally to either method.

The differential equation which is an approximation

to (B1) is, of course just (3.5a)

$$(Q/3)(dm_1/dE) = (1-r)E_R(dm_0/dE) - rm_0(E)$$
 (B2)

whose solution for m_0 , regarding m_1 as known, is

$$m_0(E) = -A \int_E^\infty dx e^{-B(x-E)} \frac{dm_1}{dx}$$
 (B3a)

$$A = Q/[3E_R(1-r)], B = r/[E_R(1-r)].$$
 (B3b)

From the solution (B3a) one may reconstruct (B1), the original difference equation.

$$\frac{Q}{3} \frac{dm_1}{dE} = -A \left[(1-r)e^{BE_R} - 1 \right] \int_E^{\infty} \left[dx e^{-B(x-E)} \frac{dm_1}{dx} \right] + A (1-r)e^{BE_R} \int_E^{E+E_R} \left(dx e^{-B(x-E)} \frac{dm_1}{dx} \right). \quad (B4)$$

It is now evident that a choice better than (B3b) is to

$$(1-r)\exp(BE_R) = 1 \tag{B5}$$

for then Eq. (B4) becomes

$$\frac{Q}{3}\frac{dm_1}{dE} = A \int_{R}^{E+E_R} dx e^{-B(x-E)} \frac{dm_1}{dx}.$$
 (B6)

This equation, in contrast to (B4), involves dm_1/dx only in the neighborhood of x=E. Ignoring the variation of dm_1/dx in the range $E < x < E + E_R$ is the only approximation and is equivalent to the Taylor's expansion to lowest order. It casts (B6) into the form

$$\frac{Q}{3}\frac{dm_1}{dE} = -A\frac{dm_1}{dE}[1 - \exp(-BE_R)]/B.$$

Hence, the best choice for A is

$$A = OB/\{3\lceil 1 - \exp(-BE_R)\rceil\}. \tag{B7}$$

The choices (B5) and (B7), when written to exhibit A and B, are

$$A = (Q/3E_R)(1/r) \ln[1/(1-r)] B = 1/E_R \ln[1/(1-r)].$$
 (B8)

Now, if the equivalent phonon energy E_R^* is defined by

$$E_R^* = \{ [(1-r)^{-1} - 1] / \ln(1-r)^{-1} \} E_R,$$
 (B9)

then Eqs. (B8) become

$$A = O/\lceil 3E_R^*(1-r) \rceil$$
, $B = r/\lceil E_R^*(1-r) \rceil$. (B10)

That is, replacing E_R^* by E_R in the differential Eq. (B2) leads to the solution (B3a) in which the constants A and B are given by (B8).

The same result can also be obtained by exact iteration of the original difference equation followed by the approximation of ignoring the variation of dm_1/dx in the interval $E < x < E + E_R$.