Solution of a new nonlinear equation for the distribution of charge carriers in a semiconductor

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The solution of a recently obtained nonlinear differential equation for the distribution function of charge carriers in a semiconductor in an electric field is derived. It is given by $f_{SL}(x)=\{1+B[s/(x+s)]^s e^x\}^{-1}$. This solution represents the symmetric part of the total distribution function. The nondimensional energy and applied electric field are x and $\sqrt{s}$, respectively, and B is a constant determined by normalization. The total distribution is given by the above and its derivative and is found to be rotationally symmetric about the electric field. This distribution reduces to the shifted Fermi-Dirac distribution for small s and to the Druyvesteyn distribution in the classical limit. An analytic expression for electrical conductivity is derived together with an approximate expression for the chemical potential in the small-electric-field limit. A generalized criterion for the classical versus quantum domains is discussed relevant to the present study. It is found that otherwise quantum domains become classical for sufficiently large applied electric fields.

I. INTRODUCTION

In a recent work by the authors[1] the kinetic theory of transport of charge carriers in a semiconductor in the presence of an electric field was addressed based on the Uehling-Uhlenbeck quasiclassical generalized Boltzmann equation.[2] The kinetic analysis was performed incorporating charge-carrier scattering with optical and acoustic phonons through strain and polar interactions.[3–5] A closed kinetic equation for the distribution of charge carriers was obtained. In steady state and passing to the classical limit, it was found that the acoustic-strain interaction dominates over remaining terms. Further assuming small phonon to charge-carrier momentum resulted in an equation which includes quantum exclusion effects and is a generalization of that found previously by Yamashita and Watanabe.[6]

In the present work this nonlinear equation is studied and it is found possible to separate the equation into two components. These components contain, respectively, quantum and electric field effects. The relation so written permits a first integral of the equation to be obtained. This integration reduces our equation to a first-order nonlinear equation which is readily reduced to quadrature.

Numerical integration is used to normalize the resulting distribution so that it represents the mean number of carriers in a single-particle state. The distribution so obtained is found to be consistent with the exclusion principle and in this regard is more appropriate to quasiclassical transport than the previously employed Druyvesteyn distribution.[7]

Passing to various limits, the distribution function reduces to well-known forms. Thus, for example, the limit of small electric field gives the displaced Fermi-Dirac distribution,[8] whereas the classical limit yields the Druyvesteyn distribution.[7]

Application is made to the construction of an expression for the conductivity of charge carriers in a semiconductor. Numerical integration of this expression returns the well-known properties that conductivity is constant at low field and falls off as $E^{-1/2}$ for high electric field. An approximate expression is obtained for the chemical potential in the limit of small electric field.

A complete analysis of our starting differential equation is included which indicates that the general solution is a function of three arbitrary constants.

II. THE DISTRIBUTION AND ITS PROPERTIES

A. Starting equation

The distribution function obtained in Ref. 1 is given by

$$f(\mathbf{k})=f_0(k)+(\cos\theta)f_1(k) \tag{1}$$

and satisfies the coupled equations

$$\frac{\partial f_0}{\partial t}+\frac{eE}{3\hbar}\left[\frac{\partial}{\partial k}+\frac{2}{k}\right]f_1=\hat{J}(f_0)\ ,$$

$$\frac{\partial}{\partial t}f_1+\frac{eE}{\hbar}\frac{\partial f_0}{\partial k}=-\frac{f_1}{\tau}\ .$$

In these equations E is electric field, e is charge, $\hbar\mathbf{k}$ is momentum, and the collision time τ is given by

$$\tau=\frac{ml}{\hbar k}\ , \tag{1a}$$

where l is mean free path.[3] The angle between **E** and **k** is denoted by θ. The collision integral has been written $\hat{J}(f_0)$.

Passing to steady state and employing expressions for $\hat{J}(f_0)$ given in Ref. 1, we obtain

$$(x+s)f_0''+\left[2+\frac{s}{x}+x(1-2af_0)\right]f_0'+2f_0(1-af_0)=0\ , \tag{2}$$

where

$$x \equiv \frac{\hbar^2 k^2}{2mk_B T}, \quad s \equiv \frac{(eEl)^2}{6mu^2 k_B T} , \tag{2a}$$

m is effective mass, T is crystal temperature, and u represents constant acoustic-phonon velocity, which is assumed to obey the inequality

$$u \ll \left[\frac{k_B T}{m} \right]^{1/2} . \tag{2b}$$

The parameter a represents exclusion effects and takes the value 1 in the quantum domain. As will be shown below; in the classical domain this term may be neglected. Setting $a=0$ in (2) returns the linear equation of Yamashita and Watanabe.[6]

The distribution (1) has the normalization

$$\frac{V}{(2\pi)^3} \int d\mathbf{k} f(\mathbf{k}) = \frac{V}{\lambda_d^3} \int_0^\infty \frac{2}{\sqrt{\pi}} f_0(x) \sqrt{x}\, dx = N \tag{3}$$

or, equivalently,

$$\int f_0(x) \sqrt{x}\, dx = \frac{\sqrt{\pi}}{2} \Lambda , \tag{3a}$$

$$\Lambda \equiv n \lambda_d^3 . \tag{3b}$$

The parameter

$$\lambda_d^2 = \frac{2\pi\hbar^2}{mk_B T} \tag{3c}$$

is the thermal deBroglie wavelength.

In writing the normalization (3) we have taken note of the fact that substitution of (1) into the left-hand side of (3) eliminates the $\cos\theta$ term in (1).

Note that $f(\mathbf{k})$ given by (1) has the alternative form

$$f(\mathbf{k}) = \left[1 - \frac{mu\lambda_d}{\hbar} \left[\frac{3s}{\pi} \right]^{1/2} (\cos\theta) \frac{\partial}{\partial x} \right] f_0(x) . \tag{4}$$

The normalization (3) implies that $f(\mathbf{k})$ represents the mean single-particle occupation number per $\mathbf{k}$ state.

B. Technique of solution

Consider the form

$$g \equiv f_0' + f_0(1 - a f_0) . \tag{5}$$

The general solution to the equation $g=0$ is the Fermi-Dirac distribution (with $a=1$)

$$f_0(x) = f_{\mathrm{FD}}(x) \equiv \frac{1}{a + B_0 e^x} , \tag{6}$$

where

$$B_0 = \exp(-\mu_0 / k_B T) , \tag{6a}$$

and μ_0 is equal to the chemical potential for $s=0$. The constant B_0 is determined through the normalization (3).

With (5) at hand, (2) may be rewritten

$$xg' + 2g + s \left[f_0'' + \frac{f_0'}{x} \right] = 0 , \tag{7}$$

or, more concisely,

$$(x^2 g)' + s(x f_0')' = 0 . \tag{8}$$

Integrating (8) gives

$$x^2 g + s x f_0' = C_1 , \tag{9}$$

where C_1 is a constant. At $x=0$ we find $C_1=0$, provided that f_0' and f_0 are finite at the origin. [For $C_1 \neq 0$, (9)

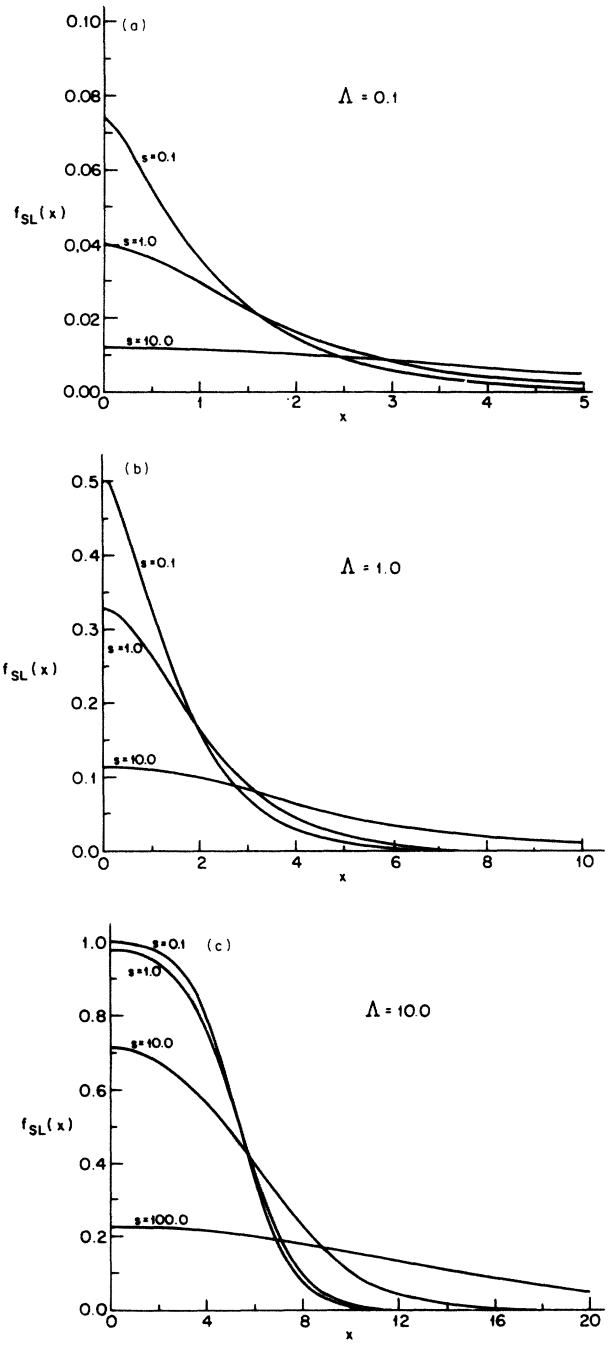

FIG. 1. $f_{\mathrm{SL}}(x)$ at varying values of s. (a) $\Lambda=0.1$, (b) $\Lambda=1.0$, and (c) $\Lambda=10.0$.

may be reduced to the Riccati equation; see Appendix A.] With this choice of C_1, rewriting (9) in explicit form gives

$$(x+s)f_0'+xf_0(1-af_0)=0 . \tag{10}$$

This equation may be reduced to quadrature and we obtain (see Appendix B)

$$f_0(x)=f_{SL}(x)\equiv\frac{1}{a+Be^x[s/(x+s)]^s} , \tag{11}$$

where B is a constant of integration and we have labeled the solution to (2), $f_{SL}(x)$, for comparison with the Fermi-Dirac distribution, $f_{FD}(x)$, and the Druyvesteyn distribution,[7]

$$f_D(x)\equiv B^{-1}e^{-x}\left[\frac{x+s}{s}\right]^s \tag{12}$$

where $x=\mathscr{E}/k_BT$, with $\mathscr{E}$ equal to the classical kinetic energy (see Appendix C).

In Fig. 1 the function $f_{SL}(x)$ is plotted for various values of the quantum and electric field parameters Λ and s. We attribute the flattening of $f_{SL}(x)$ at large s to the gain in energy of charge carriers from the electric field.

C. Limiting forms of $f_{SL}(x)$

From the normalization (3) we find that, for $s\to 0$,

$$\Lambda=\frac{2}{\sqrt{\pi}}\int_0^\infty dx\frac{\sqrt{x}}{a+Be^x} . \tag{13}$$

The property $B(s=0)\neq 0$ stems from the condition that the integral in (13) remains bounded. Numerical integration at $\Lambda=1$ [see Fig. 2(a)] gives the approximate form, for $s<1$,

$$B(s)\simeq B_0+B_1s^d=0.70+1.3s^{0.77} , \tag{14}$$

which identifies the constants B_0, B_1, and d. Substituting the resulting form for $f_{SL}(x)$ into (1) and keeping terms of $O(s^{1/2})$ returns the well-known shifted Fermi-Dirac distribution[8]

$$f(\mathbf{k})=\left[1-\frac{\tau eE}{\hbar}(\cos\theta)\frac{\partial}{\partial k}\right]f_{FD}(k) . \tag{15}$$

Next, we observe that differentiation of f_{SL} gives the property

$$f_{SL}'(x)\leq 0 , \tag{16}$$

the equality occurring only when $x=0$. It follows from (16) that

$$f_{SL}(x)_{max}=f_{SL}(0) . \tag{17}$$

We rewrite (3) as

$$\int_0^\infty f_{SL}(x)\sqrt{x}\,dx=\frac{\sqrt{\pi}}{2}\Lambda . \tag{18}$$

In that the integrand of the preceding integral is positive, we see that the classical limit,[9] $\Lambda\ll 1$, is obtained provided that $f_{SL}(x)\ll 1$. Since a is a fixed parameter in $f_{SL}(x)$, in order to attain this limit it is necessary for the B term in (11) to be large compared to a. Thus we find

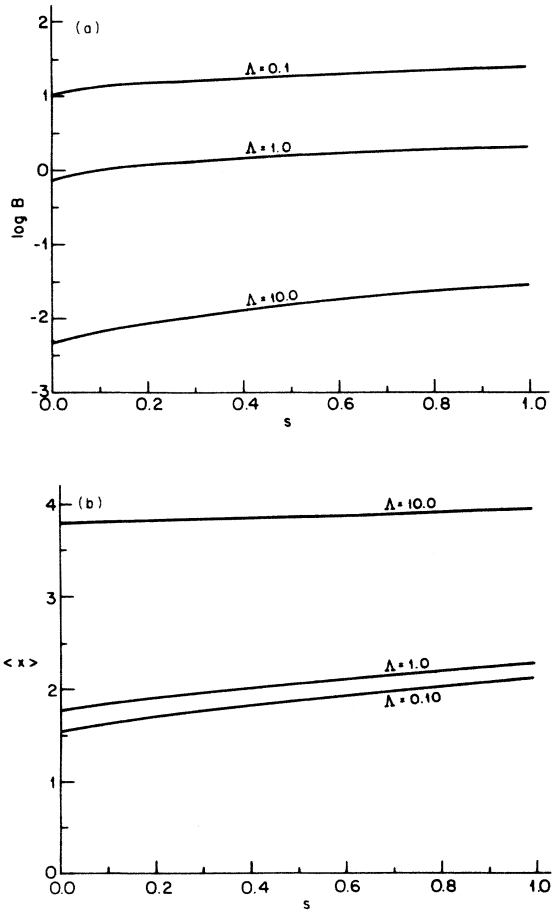

FIG. 2. (a) B vs s for $\Lambda=0.1$, 1.0, and 10.0. (b) $\langle x\rangle$ vs s for $\Lambda=0.1$, 1.0, and 10.0.

that in the classical limit

$$f_{SL}(x)=f_D(x) , \tag{19}$$

which further lends to the consistency of $f_{SL}(x)$.

D. Approximate expression for chemical potential

In the domain $s\ll 1$ we assume that (6a) is still valid. With (11) this gives the generalized chemical potential

$$\frac{-\mu}{k_BT}=\ln\left[B\left[\frac{s}{\langle x\rangle+s}\right]^s\right] . \tag{20}$$

Here we have written $\langle x\rangle$, for a nondimensional single-particle energy,

$$\langle x\rangle=\frac{2}{\sqrt{\pi}\Lambda}\int_0^\infty x^{3/2}f_{SL}(x)dx . \tag{21}$$

Evaluation of this parameter at $\Lambda=1$ gives the form [for $s<1$; see Fig. 2(b)]

$$\langle x\rangle=\langle x\rangle_0+bs^w$$
$$\langle x\rangle_0\simeq 1.76,\quad b\simeq 0.52,\quad w=0.88 . \tag{22}$$

Expanding μ as given by (20) about $s=0$ and dropping terms smaller than $O(s)$, we obtain

$$\mu=\mu_0-k_BT\left[\frac{B_1}{B_0}s^d+s\ln(s/\langle x\rangle_0)\right]. \tag{23}$$

Note that this relation has the correct limiting value, $\mu\sim\mu_0$ as $s\sim 0$.

III. CONDUCTIVITY COEFFICIENT

In this section we obtain an expression for the electrical conductivity relevant to charged carriers in a semiconductor stemming from our solution (11). With the normalization of $f(\mathbf{k})$ given by (3), the current density $\mathbf{J}$ is written

$$\mathbf{J}=e\int\frac{\hbar\mathbf{k}}{m}f(\mathbf{k})\frac{d\mathbf{k}}{(2\pi)^3}. \tag{24}$$

Substituting (1) into (24) gives

$$\mathbf{J}=e\int\frac{\hbar\mathbf{k}}{m}\left[1-\frac{\tau eE}{\hbar}(\cos\theta)\frac{\partial}{\partial k}\right]f_0(k)\frac{d\mathbf{k}}{(2\pi)^3}. \tag{25}$$

Since $f_0(k)$ is symmetric, the first term in (25) vanishes. Recalling (1a), we write

$$\mathbf{J}=\frac{-e^2El}{\hbar}\int\int\int\frac{\mathbf{k}}{k}(\cos\theta)\frac{\partial}{\partial k}f_0(k)\frac{d\phi\,d(\cos\theta)k^2dk}{(2\pi)^3}. \tag{26}$$

With $\mathbf{E}$ in the polar direction ($\theta=0$), and returning to x dependence, we find that $\mathbf{J}$ lies in the $\mathbf{E}$ direction. There results

$$\mathbf{J}=-\frac{2}{3}\frac{e^2l\mathbf{E}}{\hbar\pi\lambda_d^2}\int_0^\infty dx\,x\frac{\partial}{\partial x}f_{\mathrm{SL}}(x). \tag{27}$$

Integrating by parts gives the conductivity coefficient

$$\sigma=\sigma_0\int_0^\infty f_{\mathrm{SL}}(x)dx,\qquad \sigma_0\equiv\frac{2e^2l}{3\hbar\pi\lambda_d^2}. \tag{28}$$

Note that σ as given above is dependent on electric field through the s dependence in $f_{\mathrm{SL}}(x)$. A numerical plot of σ vs E is shown in Fig. 3. It has been previously noted[10] that, for small s, $\sigma\simeq$const. This property is evident from Fig. 3 to be valid for $s\lesssim 1$. Furthermore, for $s>1$, the numerical evaluation of (28) gives

$$\sigma\propto E^{-0.5}, \tag{29}$$

which is the observed dependence of conductivity on electric field.[3,10,11]

IV. BEHAVIOR OF PARAMETERS

We wish at this point to return to the behavior of parameters in the classical and quantum domains relevant to

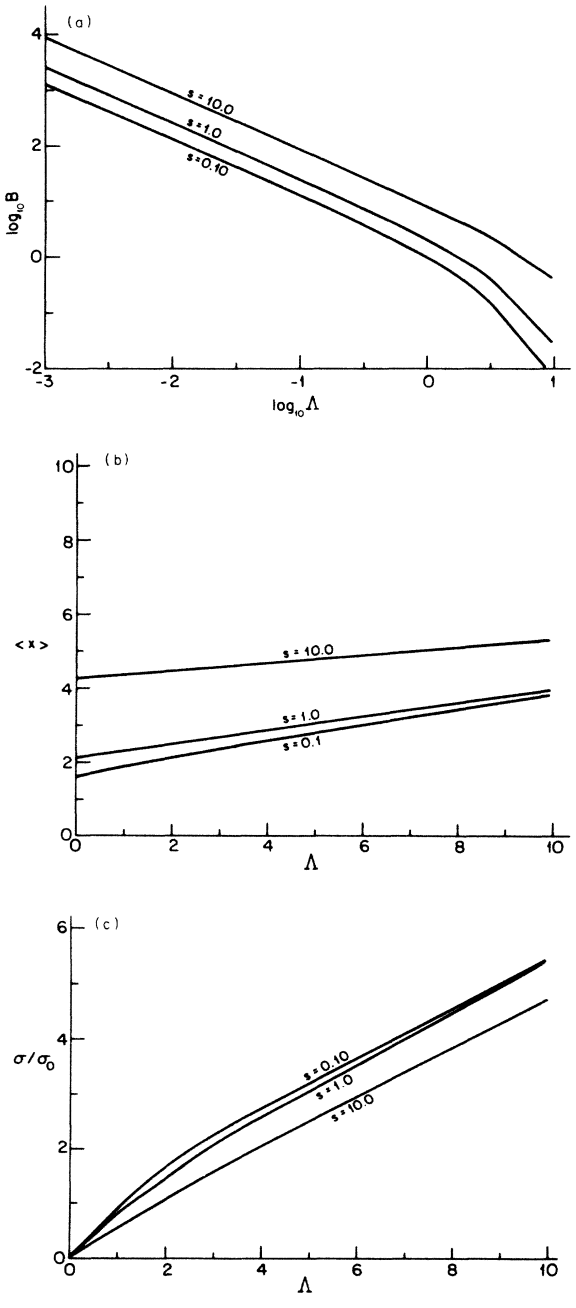

FIG. 4. The parameters (a) B, (b) $\langle x\rangle$, and (c) σ/σ_0 vs Λ.

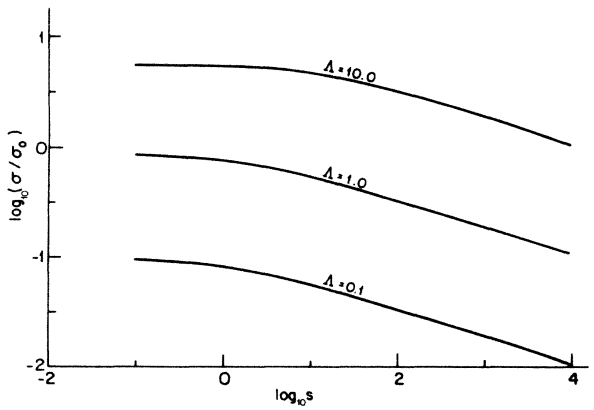

FIG. 3. Conductivity σ vs s at $\Lambda=0.1$, 1.0, and 10.0.

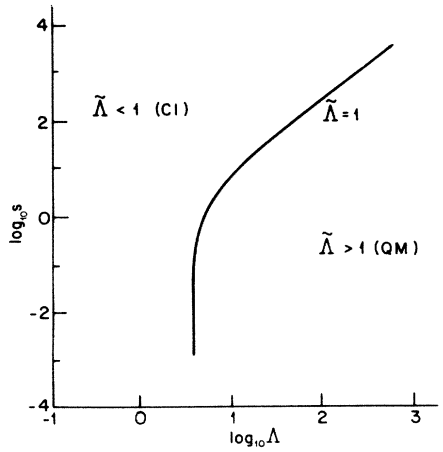

FIG. 5. Separation of classical and quantum domains in terms of $\tilde{\Lambda}$.

the distribution (11). Together with the normalization (3), at constant s, in the classical domain this distribution implies

$$B \propto \Lambda^{-1} \tag{30a}$$

and

$$\langle x \rangle \simeq \text{const} . \tag{30b}$$

With (24), still at constant s,

$$\sigma/\sigma_0 \propto \Lambda . \tag{30c}$$

These limiting properties are exhibited in Fig. 4. Note, in particular, that with $s=0$ and (30a), we obtain the classical result

$$\langle x \rangle = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-x} x^{3/2} dx = \tfrac{3}{2} , \tag{31}$$

which from Fig. 4(b) we see to be the value for $\Lambda = s = 0$.

Concerning the quantum domain, it is important to note the following. Since there is an electric field present in the medium, charge carrier energy is modified by the field. In this event, in place of the thermal deBroglie wavelength (3c), we define

$$\tilde{\lambda} = \left[\frac{2\pi\hbar^2}{m\langle \mathscr{E} \rangle} \right]^{1/2} = \langle x \rangle^{-1/2} \lambda_d . \tag{32}$$

The modified quantum parameter then becomes

$$\tilde{\Lambda} = n\tilde{\lambda}^3 = \langle x \rangle^{-3/2} n\lambda_d^3 = \frac{\Lambda}{\langle x \rangle^{3/2}} . \tag{33}$$

The quantum domain is then given by

$$\tilde{\Lambda} \gtrsim 1 . \tag{34}$$

The separation of quantum and classical behavior according to this rule is shown in Fig. 5. Note, in particular, that classical behavior at large Λ may still ensue, provided that s is sufficiently large. Thus, for example, for $\Lambda \simeq 10^2$, classical dynamics still occurs, provided that $s \gtrsim 10^3$, since for these values $\tilde{\Lambda} \lesssim 1$.

V. CONCLUSIONS

The problem of finding the distribution of charge carriers in a semiconductor in the presence of an electric field was addressed. A closed solution was derived for a previously obtained nonlinear second-order differential equation. This equation is a generalization to the degenerate domain of that found previously by Yamashita and Watanabe.[6] The technique of solution involved rewriting the equation in terms of differential functionals. This transformation allowed reduction of the equation to a perfect differential form, which, in turn, was integrated to yield a first-order equation. The solution was then obtained through integration of this reduced form.

The derived solution reduces to the Druyvesteyn distribution[7] in the nondegenerate domain and the displaced Fermi-Dirac distribution for small values of electric field.

A closed expression for electrical conductivity was obtained. Numerical integration of this expression showed saturation of conductivity at sufficiently large electric field, and otherwise agreement with experimental values.

Plots of numerical results were also made of the distribution function and its parameters. An approximate expression for the chemical potential was obtained for small electric field, which was found to reduce to the correct form at zero electric field.

It should be noted that the important topic of "hot" electron transport[12] (i.e., high energy relative to crystal temperature) in a semiconductor is described in the present work by $\langle x \rangle \gg 1$, since temperature as contained in x [see (2a)] is crystal temperature. An equivalent criterion is given by $\tilde{\Lambda}/\Lambda \ll 1$ [see (33) and Fig. 5].

ACKNOWLEDGMENTS

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APPENDIX A: GENERAL SOLUTION

Dropping the subscript on f_0, (9) becomes

$$f' + \frac{x}{x+s} f(1-af) = \frac{C_1}{x(x+s)} . \tag{A1}$$

With the identifications

$$P \equiv \frac{x}{x+s}, \quad Q \equiv -\frac{C_1}{x(x+s)}, \quad R \equiv -aP , \tag{A2}$$

(A1) becomes

$$f' + Pf + Q + Rf^2 = 0 , \tag{A3}$$

which we recognize to be the Riccati equation.[13,14] This equation may be reduced to linear form through the transformation

$$f = \frac{(\ln y)'}{R} . \tag{A4}$$

There results

$$y''+\left[P-\frac{R'}{R}\right]y'+(QR)y=0\ , \tag{A5}$$

where

$$P-\frac{R'}{R}=\frac{x^2-s}{x(x+s)},\quad QR=\frac{C_1 a}{(x+s)^2}\ . \tag{A6}$$

Thus the general solution to (A5) may be written as a linear combination of two independent solutions. For the case at hand, since the coefficient of y' has a simple pole at the origin, and QR has, at most, a double pole at the origin, we may conclude[15] that the general solution to (A5) may be written as an arbitrary linear combination of two Frobenius series about the origin.

Note, in particular, that with C_1, the solutions to (A6) contain three arbitrary constants. We may conclude that the solutions to our starting equation, (2), are likewise given in terms of three arbitrary constants.

For $a=0$, (2) is linear. In this event, (A1) is also linear and yields only one additional constant of the motion. With C_1 this comprises a total of two constants of the motion for the general solution to the starting equation (2) in the classical domain.

APPENDIX B: SOLUTION TO THE REDUCED EQUATION

We recall (10) (and delete the subscript 0),

$$(x+s)f'+xf(1-af)=0\ . \tag{B1}$$

Integrating, we obtain

$$\int_{f(x_0)}^{f}df\frac{1}{f(1-af)}=-\int_{x_0}^{x}\frac{x}{x+s}dx\ , \tag{B2}$$

which gives

$$\ln\left|\frac{f}{1-af}\right|=-x+s\ln\left|\frac{x+s}{s}\right|-\ln B\ , \tag{B3}$$

where $\ln B$ contains constants of integration. Taking the exponential of (B3) gives the desired result (11).

APPENDIX C: RELATION TO THE CLASSICAL DRUYVESTEYN DISTRIBUTION

In this appendix we wish to relate the form (12) with the common expression for the Druyvesteyn distribution[16] relevant to charged particles of mass m moving through a medium of neutral particles of mass $M\gg m$ in the presence of an electric field. It is given by

$$f_D(c)=A\exp\left[-\int_0^c dc\frac{mc}{k_BT+Me^2E^2l^2/(3m^2c^2)}\right], \tag{C1}$$

where c is charge-particle velocity. Defining the speed α by

$$\alpha^2=\frac{M}{3k_BT}\left[\frac{eEl}{m}\right]^2 \tag{C2}$$

permits the preceding to be written

$$f_D(c)=A\exp\left[-\frac{m}{k_BT}\int_0^c dc\frac{c^3}{c^2+\alpha^2}\right]. \tag{C3}$$

With α constant, integration gives

$$f_D(x)=A'e^{-x}\left[\frac{x+\tilde{s}}{\tilde{s}}\right]^{\tilde{s}}, \tag{C4}$$

where

$$x\equiv\frac{mc^2}{2k_BT},\quad \tilde{s}=\frac{m\alpha^2}{2k_BT}\ . \tag{C5}$$

Comparing (C4) with (12), and with reference to (2a), we obtain the correspondence

$$u^2=\frac{k_BT}{M}\ . \tag{C6}$$

This equation relates the phonon speed u with the thermal velocity of the background medium, k_BT/M. Note, in particular, that with (C6) and (2b),

$$\frac{k_BT}{M}=u^2\ll\frac{k_BT}{m}\ ,$$

which is consistent with the starting assumption $M\gg m$.

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