PHYSICAL REVIEW B VOLUME 22, NUMBER 2 15 JULY 1980

Electron mobilities based on an exact numerical analysis of the dielectric-function-dependent linearized Poisson's equation for the potential of impurity ions in semiconductors

L. M. Scarfone
Department of Physics, University of Vermont, Burlington, Vermont 05401

Llanda M. Richardson
Digital Equipment Corporation, Westboro, Massachusetts 01581

(Received 17 August 1979)

The complete linearized Poisson's equation for the impurity-ion potential incorporating the spatial variation of the semiconductor dielectric function is treated numerically as a boundary-value problem with the finite-difference method. The impurity-ion potential so derived is shown by direct substitution to be a superior solution to the differential equation than that obtained by an equivalent variational-principle approach, or by the straightforward replacement of the dielectric constant by the dielectric function of the Dingle potential. Theoretical electron mobilities for silicon, germanium, and gallium arsenide based on this potential are compared with the Dingle mobility. It is found that the result of including the spatial variation of the dielectric function in the theory of ionized-impurity scattering is to reduce the electron mobility from that calculated using the Dingle potential. This effect is small, except in the cases of heavy and very heavy doping, where it is found that the difference increases monotonically as the doping density is likewise increased.

I. INTRODUCTION

The scattering of mobile charge carriers by ionized impurities in a doped semiconductor at finite temperatures has been widely studied in terms of the Born-approximation theory of Brooks and Herring[1] (BH). A less rigorous semiclassical treatment given earlier by Conwell and Weisskopf[2] (CW) considers the same physical problem in terms of Rutherford scattering. The BH formalism is distinguished by a self-consistently determined screened Coulomb potential which incorporates the electrostatic shielding of a (point) impurity ion by the mobile carriers that collect around the ion and also by the other static ionized impurities. Depending on whether the carriers are described by quantum or classical statistics, the shielding parameter is generally called the Thomas-Fermi[3] or Debye-Hückel[4] screening length, respectively. Screening effects in the CW approach are simulated by arbitrarily cutting off the scattering cross section at a radial distance equal to half the average separation between neighboring ionized impurities.[5] In the nondegenerate regime, providing the carrier concentration coincides with the concentration of ionized impurities, both theories yield essentially the same results for ionized-impurity-scattering limited mobility. However, when the carrier concentration is less than that of the ionized impurities, only the BH theory accounts for the decrease in screening and predicts a smaller carrier mobility, as expected.[6]

While the BH and CW theories give qualitatively correct results, there are refinements by which they may be improved. One of these refinements is of current interest and involves a more accurate description of dispersive valence screening. The dielectric response of the valence electrons to the pure Coulomb field of CW or to the screened Coulomb field of BH is accounted for in these theories simply through scaling by the static dielectric constant κ_0 of the semiconducting medium. In the very recent literature, two quite different schemes have been proposed for generalizing the BH theory of screening to include more realistic valence screening effects. Both approaches generalize Dingle's[1] form of the BH theory. It also seems worthwhile to consider similar extensions of the CW theory for comparison. This problem is presently under investigation.

In a previous paper,[7] we used a variational-principle procedure to obtain an approximate solution of the complete linearized Poisson's equation describing an impurity-ion potential which includes these more accurate valence-screening effects. Here, we present a purely numerical approach to the problem of solving this equation.[8] The resulting potential is compared and contrasted with that developed in Ref. 7, and with the standard Dingle potential. Electron mobilities corresponding to the new potential and the Dingle potential are displayed graphically for silicon, germanium, and gallium arsenide over a wide range of electron concentrations at $T = 300$ K. Except for the case of heavy doping, very little difference is found between the mobility including dispersive valence-screening effects and the standard Dingle mobility. The discrepancy between this finding and the conclusion in Ref. 7 concerning a similar comparison is believed to be due to an approximation made in the variational calculation.

II. TEMPERATURE-DEPENDENT IMPURITY-ION POTENTIALS INCLUDING DISPERSIVE VALENCE-SCREENING EFFECTS

A. Local linear-response theory

The first attempt at generalizing Dingle's model of the screening of impurity ions in doped semiconductors at nonzero temperature by incorporating valence-screening effects beyond those carried by the static dielectric constant is due to Csavinsky.[9] He proposes the Poisson equation

$$\phi'' + \frac{2}{r}\phi' + \frac{4\pi\rho}{\kappa(r)} = -\frac{\kappa'(r)}{\kappa(r)}\phi , \qquad (1)$$

for the impurity-ion potential $\phi(r)$. Here ρ denotes the free-carrier screening charge density, while $\kappa(r)$ is the so-called spatial dielectric function, conventionally defined as the ratio of the unscreened potential due to the point probe charge to the effective potential ϕ modified by the screening effects. In the linear approximation, ρ is given by

$$\rho = -(\kappa_0/4\pi R_0^2)\phi(r) , \qquad (2)$$

where R_0 the Dingle screening length depends on the impurity concentration n_i, the carrier effective mass m, and the temperature T. Equation (1) is rooted in an assumed local algebraic generalization

$$\vec{\mathrm{E}}(r) = \kappa^{-1}(r)\vec{\mathrm{D}}(r) , \qquad (3)$$

of the usual macroscopic constitutive relation between the electric displacement vector $\vec{\mathrm{D}}$ of the point charge and the screened electric field $\vec{\mathrm{E}}$. The approximate analytical form of $\kappa^{-1}(r)$ used by Csavinsky for silicon[10] and germanium,[11] namely,

$$\kappa^{-1}(r) = \kappa_0^{-1} + e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r} , \qquad (4)$$

is based on the fit of a five-parameter function to the wave-vector-dependent dielectric function $\epsilon(k)$, evaluated numerically within the context of the homogeneous and isotropic model semiconductor of Penn.[12] The parameters α, β, γ, A, and B are constants specific to a given semiconductor and are tabulated in Refs. 10 and 11.

Approximate solutions of the linearized version of Eq. (1), with the neglect of the right-hand side, have been formulated in terms of an equivalent variational principle.[9] These potentials are conveniently but arbitrarily taken to be linear combinations of two screened Coulomb potentials with either two parameters n and C, or one parameter, a, to be determined numerically from the variational calculations. In the former case

$$\phi_1(r) = \phi_0(r)[Ce^{nr/R_0} + (1 - C)e^{-nr/R_0}] , \qquad (5)$$

while in the latter

$$\phi_2(r) = \phi_0(r)[1 + (\kappa_0 - 1)e^{-ar}] . \qquad (6)$$

Calculations of ionized-impurity limited mobility based on ϕ_1 and ϕ_2 yield results that, respectively, either overestimate[13] or grossly underestimate[14] the mobility based on the standard Dingle potential ϕ_0. In a subsequent development, Richardson and Scarfone,[7] making use of a functional devised by Brownstein,[15] obtained an approximate solution of the complete linearized Poisson equation. The potential ϕ_3 (in Ref. 7, ϕ_3 was referred to simply as ϕ) was chosen to have the form exhibited in Eq. (6) and gives an accurate account of valence dielectric screening as proposed by Csavinsky.[9] The corresponding mobility[7] is a meaningful improvement over the Dingle mobility and over previous treatments[13,14] of the problem.

As previously noted, the particular form of $\kappa(r)$ appearing in Eq. (4) is founded on fitting a specific five-parameter function to a calculated $\epsilon(k)$. Whether one employs the Penn model, or some other description of $\epsilon(k)$, the continued use of this approach entails a cumbersome fitting procedure for each semiconductor of interest. Because $\epsilon(k)$ in the simple Penn model alrealy involves complicated integrations in k space, it is understandable that even simpler theories[16] of dielectric screening are sought, and that various analytical interpolation formulae have been advanced in the literature[17] to represent the linear response in k space, or its spatial equivalent, in applications.

B. Nonlocal linear-response theory

A different scheme also aimed at modifying valence-screening effects in the Dingle model has been forwarded by Resta,[18] who deals with an integro-differential Poisson equation,

$$\nabla^2\phi - R_0^{-2}\kappa_0 \int \epsilon^{-1}(|\vec{\mathrm{r}} - \vec{\mathrm{r}}'|)\phi(\vec{\mathrm{r}}')d\vec{\mathrm{r}}' = -4\pi e_0\epsilon^{-1}(r) , \qquad (7)$$

for the case of a point probe charge e_0 in the usual homogeneous and isotropic model semiconductor. Equation (7) implies that the linear response of the valence electrons to the point perturbation is nonlocal in r space. In this theory the convolution integral

$$\vec{\mathrm{E}}(\vec{\mathrm{r}}) = \int \epsilon^{-1}(|\vec{\mathrm{r}} - \vec{\mathrm{r}}'|)\vec{\mathrm{D}}(\vec{\mathrm{r}}')d\vec{\mathrm{r}}' \qquad (8)$$

plays a central role. It is obvious from Eqs. (3) and (8) that these expressions of dielectric behavior are on completely different conceptual footings. While both theories assume a linear relationship between the screened electric field and the displacement vector, Eq. (3) is a local algebraic relationship invoking the spatially variable dielectric function κ, whereas Eq. (8) is a nonlocal operation involving the linear response ϵ^{-1}. This fundamental difference between the two schemes has been stressed by Resta.[18]

The solution of Eq. (8) may be stated in the form

$$\phi_R(r)=\frac{2e_0}{\pi r}\int_0^\infty \frac{k\sin kr\,dk}{k^2\epsilon(k)+\kappa_0 R_0{}^{-2}}\,. \tag{9}$$

Given an expression for $\epsilon(k)$, the generalized Dingle potential in this case is determined from Eq. (9). In the previous case, the development of an ionized-impurity potential via Eqs. (1) and (2) assumes, among other things, that an analytical expression for $\kappa(r)$ has been obtained from the given $\epsilon(k)$ for each semiconductor of interest. The potential expressed in Eq. (9) has been compared with ϕ_0 and found to be stronger only at small r.[18] This comparison was implemented in terms of Thomas-Fermi[3,16] (TF) dielectric functions $\epsilon(k)$ and $\kappa(r)$, rather than the Penn-model dielectric functions. In the former case one first finds $\kappa(r)$ and then $\epsilon(k)$ follows, while in the latter the order is reversed. The TF dielectric functions are found to be in excellent agreement with Srinivasan's[12] Penn-model calculations, and with the random-phase approximation results of Walter and Cohen.[12] The primary advantage in using the TF dielectric functions is that of having simple analytical forms to work with, not to mention that at low values of k, Penn's model is very unreliable. As in the Penn model, the only input data required for the TF dielectric functions are κ_0 and the valence Fermi momentum k_F.

The spatial dielectric function used by Resta to establish $\epsilon(k)$ in Eq. (9) has the simple analytical form

$$\kappa(r)=\begin{cases}\kappa_0 qR/[\sinh q(R-r)+qr], & r\leq R\\ \kappa_0, \quad r\geq R\,.\end{cases} \tag{10}$$

The quantity q in Eq. (10) is an abbreviation for $(4k_F/\pi)^{1/2}$, while R is the screening radius beyond which the screened potential of a point charge has the pure Coulomb form scaled by κ_0. Continuity of the electric field at $r=R$ provides the condition $\sinh qR/qR=\kappa_0$ for the determination of R for each semiconductor considered.

III. NUMERICAL SOLUTION OF THE LINEARIZED POISSON EQUATION BY THE METHOD OF FINITE DIFFERENCES

The approximate solution of the complete linearized Poisson's equation

$$\phi''+(2/r)\phi'+\kappa^{-1}(\kappa'-\kappa_0/R_0^2)\phi=0 \tag{11}$$

given in Ref. 7 makes use of the Azuma-Shindo dielectric function and an equivalent variational-principle procedure. Another possible method of solution is a purely numerical approach.[8] As the differential equation of interest poses a boundary-value problem, it is natural to think of using the method of finite differences.[19] The reasons for seeking another solution are twofold. First, a solution derived by alternative means will serve as a comparison for the variational calculation. Second, the algebraic manipulations necessary for the final extremalization in the variational approach are long and tedious. Thus, if we desire to obtain the impurity-ion potential using another analytical dielectric function $\kappa(r)$, we would have to either parametrize that function to have the same form as the Azuma-Shindo expression Eq. (4), or rederive the entire function F used in the equivalent variational principle,[7] and perform the subsequent calculations with some new $\kappa(r)$. A numerical approach makes the shift to another $\kappa(r)$ much less cumbersome.

The chief advantage of this complete numerical treatment is that any $\kappa(r)$ may be used without additional difficulty beyond the adjustment of a few lines in the computer program. The drawbacks of a numerical approach are first, that the potential must be solved by a separate calculation for each Dingle screening length R_0 of interest. As the curves presented in this paper use approximately fifty different values of R_0 each, this process demands a large quantity of computer time. Second, the results from the finite differences techniques are not immediately applicable to further calculations since the numbers generated by the program must first be fit to some convenient analytical function.

Dielectric functions $\kappa(r)$ considered in some detail for use here are due to Azuma and Shindo,[10] Schulze and Unger,[17] and Resta.[16] The first and third of these have been already noted in Eqs. (4) and (10), respectively. The Schulze-Unger r-dependent dielectric function is based on a simple analytical form for $\epsilon(k)$ which accounts correctly for the limiting cases $k=0$ and asymptotic large k values. For the limiting case of a metal, the screening is not allowed to be stronger than that in a free electron gas, and finally, the spatial polarization of the valence electrons around a

TABLE I. Values of the parameter t corresponding to a in Eq. (6) for the impurity-ion potential ϕ_4 for silicon.

R_0 (a.u.)	t (a.u.$^{-1}$)
10.0	2.5950
11.0	2.5972
12.0	2.5994
13.0	2.6016
14.0	2.6038
15.0	2.6060
16.0	2.6075
17.0	2.6089
18.0	2.6104
19.0	2.6118
20.0	2.6133
21.0	2.6145
22.0	2.6157
23.0	2.6170
24.0	2.6182
25.0	2.6194
30.0	2.6255
35.0	2.6252
40.0	2.6289
45.0	2.6314
50.0	2.6340
55.0	2.6358
60.0	2.6375
65.0	2.6389
70.0	2.6402
75.0	2.6411
80.0	2.6421
85.0	2.6430
90.0	2.6440
95.0	2.6441
100.0	2.6442
105.0	2.6443
110.0	2.6444
115.0	2.6446
120.0	2.6447
125.0	2.6448
130.0	2.6450
135.0	2.6451
140.0	2.6453
145.0	2.6454
150.0	2.6456
155.0	2.6458
160.0	2.6472
165.0	2.6436
170.0	2.6500
175.0	2.6501
180.0	2.6502
185.0	2.6502
190.0	2.6503
195.0	2.6503
200.0	2.6503
205.0	2.6502
210.0	2.6502
215.0	2.6505
220.0	2.6508
225.0	2.6510
230.0	2.6513

point charge should reach its full strength in a certain distance related to the nearest-neighbor distance. For silicon, the Azuma-Shindo function does not reach its static value as rapidly as do the other two. Since Srinivasan[12] has noted that the dielectric function should attain its limiting value at a distance of the order of the nearest-neighbor distance, we find this behavior unsatisfactory. On the other hand, the Schulze-Unger function displays a slight peak, overshooting the static value. Again, Srinivasan, and Vinsome and Richardson[12] have noted that overshoots of this type are generally the result of some delicate numerical imbalance and should not be endowed with any physical significance. Therefore, although the Schulze-Unger has a simple analytic form and is readily extended to any semiconductor for which κ_0 and k_F are known, we find the presence of the overshoot to be less than desirable. The Resta dielectric function in Eq. (10) does not have these various shortcomings. We use this function in our finite differences calculations because of its smooth monotonic behavior and adaptability to different semiconductors. This function leads to $\epsilon(k)$ functions with the same behavior as, and numerically quite close to, the accurate results of Walter and Cohen, as already mentioned.

It is useful to fit the numerical results from the finite differences calculation to some simple analytical expression. For this purpose, we have chosen the one-parameter form given in Eq. (6). To distinguish this potential from previous ones, we shall call it ϕ_4 and let t be the corresponding parameter. Tables I, II, and III of t as a function of R_0 for silicon, germanium, and gallium arsenide, respectively, are included. Because t varies only slightly with R_0 and the computer time necessary to generate each value of t is not insignificant, some of the t values presented are a linear interpolation between calculated values. The values listed arise from data produced under the assumption that $\phi_4 = \phi_0$ at $r = 25$ a.u. This assumption is somewhat arbitrary, but necessary in view of the fact that correspondence at infinity cannot be achieved on a computer. The total number of steps used to obtain these results is 1200.

In Fig. 1 we have graphed the three potentials ϕ_0, ϕ_3, and ϕ_4 for silicon at $R_0 = 15$ a.u., as a function of r. Note that ϕ_4 approximates ϕ_0 at a distance of about 2 a.u., whereas ϕ_3 does not approach ϕ_0 until closer to 9 a.u. That there is a discrepancy between the two solutions is probably due to the nature of an approximation[20] made in the variational solution. It is not entirely clear why the variational method failed to yield a root (extremum) without the use of this approximation. However, it did produce a potential with a more

TABLE II. Values of the parameter t corresponding to a in Eq. (6) for the impurity-ion potential ϕ_4 for germanium.

R_0 (a.u.)	t (a.u.$^{-1}$)
10.0	2.4796
11.0	2.4804
12.0	2.4812
13.0	2.4820
14.0	2.4828
15.0	2.4836
16.0	2.4848
17.0	2.4860
18.0	2.4873
19.0	2.4885
20.0	2.4897
21.0	2.4905
22.0	2.4913
23.0	2.4921
24.0	2.4929
25.0	2.4937
30.0	2.4992
35.0	2.4999
40.0	2.5028
45.0	2.5053
50.0	2.5078
55.0	2.5092
60.0	2.5106
65.0	2.5117
70.0	2.5128
75.0	2.5136
80.0	2.5140
85.0	2.5144
90.0	2.5161
95.0	2.5167
100.0	2.5170
105.0	2.5172
110.0	2.5184
115.0	2.5186
120.0	2.5187
125.0	2.5189
130.0	2.5193
140.0	2.5198
145.0	2.5199
150.0	2.5201
155.0	2.5205
160.0	2.5206
165.0	2.5203
170.0	2.5210
175.0	2.5212
180.0	2.5215
185.0	2.5217
190.0	2.5219
195.0	2.5221
200.0	2.5224
205.0	2.5226
210.0	2.5229
215.0	2.5228
220.0	2.5228
225.0	2.5227
230.0	2.5226

TABLE III. Values for the parameter t corresponding to a in Eq. (6) for the impurity-ion potential ϕ_4 for gallium arsenide.

R_0 (a.u.)	t (a.u.$^{-1}$)
10.0	2.4716
11.0	2.4732
12.0	2.4748
13.0	2.4763
14.0	2.4779
15.0	2.4795
16.0	2.4809
17.0	2.4822
18.0	2.4836
19.0	2.4849
20.0	2.4863
21.0	2.4872
22.0	2.4882
23.0	2.4891
24.0	2.4910
25.0	2.4910
30.0	2.4972
35.0	2.4975
40.0	2.5011
45.0	2.5033
50.0	2.5056
55.0	2.5074
60.0	2.5092
65.0	2.5104
70.0	2.5117
75.0	2.5126
80.0	2.5135
85.0	2.5144
90.0	2.5153
95.0	2.5156
100.0	2.5160
105.0	2.5164
110.0	2.5167
115.0	2.5172
120.0	2.5178
125.0	2.5183
130.0	2.5188
135.0	2.5191
150.0	2.5193
145.0	2.5196
150.0	2.5198
155.0	2.5200
160.0	2.5202
165.0	2.5205
170.0	2.5208
175.0	2.5210
180.0	2.5211
185.0	2.5211
190.0	2.5212
195.0	2.5212
200.0	2.5213
205.0	2.5215
210.0	2.5217
215.0	2.5219
220.0	2.5221
225.0	2.5223
230.0	2.5222

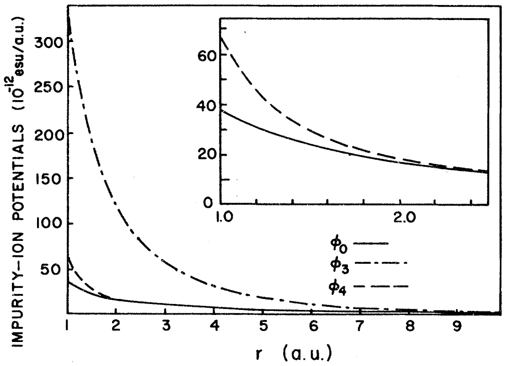

FIG. 1. Impurity-ion potentials ϕ_0, ϕ_3, and ϕ_4, as a function of the distance r from the origin. The curves are for silicon with the Dingle screening length $R_0 = 15$ a.u.

physically reasonable behavior than either ϕ_1 or ϕ_2. In any case, at this point, we feel that ϕ_4 embodies the best solution of Eq. (11) of the four impurity-ion potentials.

We may demonstrate this more explicitly by calculating the value of the differential equation for the three potentials ϕ_0, ϕ_3, and ϕ_4; that is, we seek an evaluation of the function $f(r)$ defined in terms of $\psi = (\kappa_0 r/e_0)\phi$ by

$$f(r) = \psi'' - [\kappa_0 R_0^{-2}\psi - \kappa'(\psi' - \psi/r)]\kappa^{-1} \tag{12}$$

for all three potentials. Obviously, a "perfect" solution to the differential equation will yield $f(r) = 0$. Figure 2 displays values of $f(r)$, for silicon at $R_0 = 15$ a.u., as a function of r. The crosses (squares) correspond to the function ψ_3 (ψ_4) derived from the variational (finite-differences) calculation. It is evident that, for all values of r, $f(r)$ is closest to zero for ϕ_4, rather than ϕ_3. We have also shown in Fig. 2 the values of $f(r)$ using a potential of the form

$$\phi_{\mathrm{TQ}}(r) = \frac{e_0}{\kappa(r) r}\, e^{-r/R_0}, \tag{13}$$

as proposed by Theodorou and Queisser.[13] This potential is obtained in a non-self-consistent manner by simply replacing the static dielectric constant in ϕ_0 by the spatially dependent dielectric function. In their case, which deals with compensation effects, this is justified by the low concentration of free carriers. It is seen that $|f(r)|$ for ϕ_{TQ} is greater than $|f(r)|$ for ϕ_4 at low values of r (0.75 a.u.). At larger values of r, the converse is true, and, as r increases, the values of $|f(r)|$ interchange their relationship frequently, although too slightly to be visible in Fig. 2. However, since it is the small-r region which is the most critical, it follows that the behavior of ϕ_4 there is the more satisfactory. Additionally, Fig. 2 shows the values of $f(r)$ for the Dingle potential ϕ_0. It is seen that ϕ_0 consistently yields the lowest results for $|f(r)|$. Actually, this is merely a curiosity because ϕ_0 does not satisfy the boundary condition at the origin which is necessary when spatial variation of the dielectric function is considered.

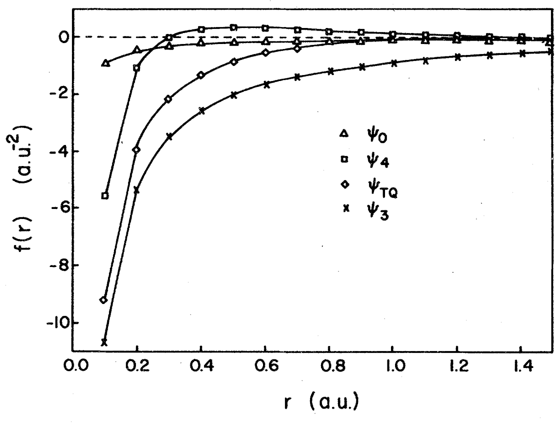

FIG. 2. Values of the differential equation $f(r)$ Eq. (12) as a function of the distance from the origin. These are plotted for the impurity-ion potential functions ψ_0, ψ_3, ψ_4, and ψ_{TQ} (omitting the common e_0 factor in all cases). The curves are for silicon at $R_0 = 15$ a.u.

Thus ϕ_4 is an impurity-ion potential which is constrained to be a factor of κ_0 times greater than ϕ_0 at the origin, but which rapidly decreases with r and approaches ϕ_0 well within a nearest-neighbor distance. The adjustment which is made in the potential by the consideration of the spatial behavior of the dielectric function is, therefore, confined to a region very close to the origin.

IV. CALCULATION OF THE CONDUCTIVITY MOBILITY

This section is concerned with the electron conductivity mobility, μ_4, arising from ϕ_4. The procedure here is the same as that used[7] for ϕ_3 and, therefore, we immediately write down an expression determining μ_4 in the first Born approximation, namely,

$$\mu_4 = \frac{8\sqrt{2}\,\kappa_0^2 (k_B T)^{3/2}}{\pi^{3/2}\eta_i e_0^3 \sqrt{m^*}}\, Q_4^{-1}(k_{\max})\, \frac{F_2(\eta)}{F_{1/2}(\eta)}, \tag{14}$$

where Q_4 is defined by

$$Q_4 = \left(\ln(1+b_0^2) - \frac{b_0^2}{1+b_0^2}\right) + (\kappa_0 - 1)^2\left(\ln(1+b_4^2) - \frac{b_4^2}{1+b_4^2}\right) + (\kappa_0 - 1)\left[\ln(b_0^2 b_4^2 + b_4^2 + b_0^2 + 1) - \left(\frac{b_0^2+b_4^2}{b_0^2-b_4^2}\right)\ln\left(\frac{1+b_0^2}{1+b_4^2}\right)\right]. \tag{15}$$

Here we have defined $b_0 = 2kR_0$ and $b_4 = 2kR_4$, where

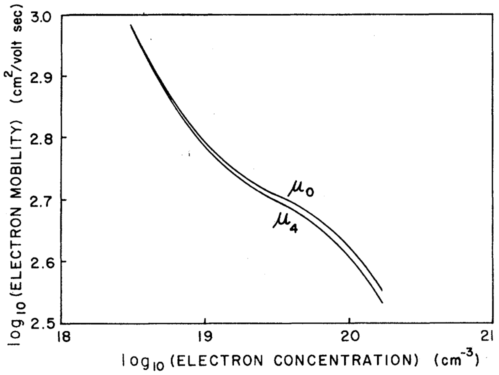

FIG. 3. Theoretical electron conductivity mobilities, μ_0 and μ_4, for silicon at $T = 300$ K as a function of electron concentration.

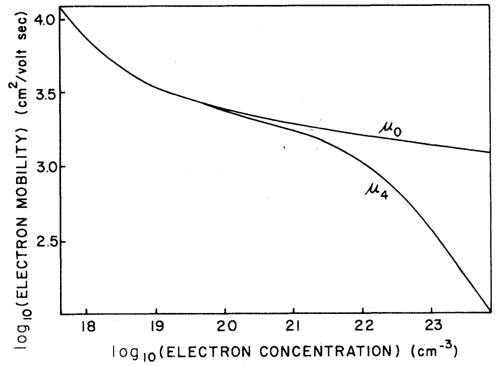

FIG. 5. Theoretical electron conductivity mobilities, μ_0 and μ_4, for gallium arsenide at $T = 300$ K as a function of electron concentration.

k is the electron wave number, and $R_4 = R_0/(1 + tR_0)$. The quantity $F_\alpha(\eta)$ is the Fermi-Dirac integral of order α, defined, for example, in Blackmore[21] as a function of the reduced chemical potential η. As usual, the derivation of Eq. (14) involves an integral that averages the relaxation time for ionized-impurity scattering over the Fermi-Dirac distribution function. Following the original technique of CW, we evaluate Q_4 in Eq. (14) at that value of k ($k_{\max}$) that maximizes the integrand remaining in this integral after the removal of $Q(k_{\max})$. Finally, k_B in Eq. (14) is the Boltzmann constant. For the particular case of the Dingle potential the corresponding mobility, μ_0 follows from Eq. (14) by retaining only the first quantity in large parentheses on the right-hand side of Eq. (15).

In Figs. 3, 4, and 5 we have graphed μ_0 and μ_4 as a function of electron concentration, which here is the same as n_i, for silicon, germanium, and gallium arsenide, respectively, at $T = 300$ K. Also in Fig. 6, the mobility ratio μ_4/μ_0 is presented as a function of electron concentration for these semiconductors at the same temperature. In the interest of a clear illustration of the difference between μ_0 and μ_4, we have not included any experimental points, as to do so would cause the vertical scale to be enlarged. Furthermore, for gallium arsenide the only points available to us did not extend into the very heavily doped region.

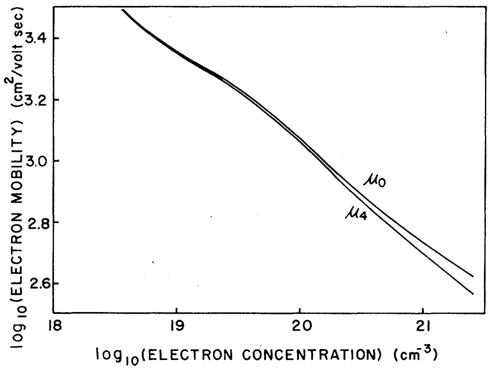

FIG. 4. Theoretical electron conductivity mobilities, μ_0 and μ_4, for germanium at $T = 300$ K as a function of electron concentration.

It is seen from these graphical results that the change in μ_4 from μ_0 is very slight, except for high levels of doping. However, the trend is in the proper direction, toward the experimental points, so that the effect of including dispersive valence-screening effects is to reduce the theoretical electron mobility resulting from ionized-impurity scattering compared with the original Dingle mobility. This is to be expected physically since ϕ_4 is much stronger than ϕ_0 in the small-r region. The deviation of μ_4 from μ_0 is much less pronounced than was the case in Fig. 4 of Ref. 7 where ϕ_3 was used. The reasons for this difference are twofold. First, for the case of silicon, we are here using a dielectric function which reaches its limiting value in approximately half the distance at which the Azuma-Shindo function reaches theirs. That is, the physical region wherein the dielectric function is not a constant has been decreased by a factor of 2. Second, and most important, we believe the discrepancy of results has its roots in the approximation[20] that was necessitated to obtain a solution in the variational approach. We would expect, without proof, that the results from the unapproximated variational approach should closely resemble those derived from the finite-differences method.

V. CONCLUDING REMARKS

We have seen that a purely numerical determination of the impurity-ion potential satisfying the linearized Poisson equation (11) provides the most accurate and efficient means of incorporating the spatial variation of the dielectric function into the theory of ionized-impurity scattering. We conclude that the electron mobility based on this potential is lower than the Dingle mobility at high impurity concentrations and approaches the latter at low doping densities. The effect is negligible for doping less than about 10^{18} cm^{-3} for silicon and germanium, and less than about 10^{19} cm^{-3} for gallium arsenide. As shown in Fig. 6, the ratio μ_4/μ_0 remains greater than 0.90 for most concentrations of interest; that is, our result, for the effect on the theoretical electron conductivity mobility calculated from a self-consistent impurity-ion potential which incorporates linear screening effects due to valence electrons and free change carriers, is that the change in the mobility from the Dingle mobility is a small effect except for cases of very heavy doping.

We wish to note that while the calculations in the present paper are based on the linearized Poisson's equation, we can also think of calculating electron mobility in terms of the nonlinear Poisson equation.[22] It is expected that nonlinear impurity screening effects will be important.

Finally, we mention that after the present work was completed, we became aware of the numerical results of Meyer.[23] His potential in the linear case, although similar to ours, was obtained using the Azuma-Shindo dielectric function which, as discussed above, is not currently the most accurate description of dispersive valence screening.

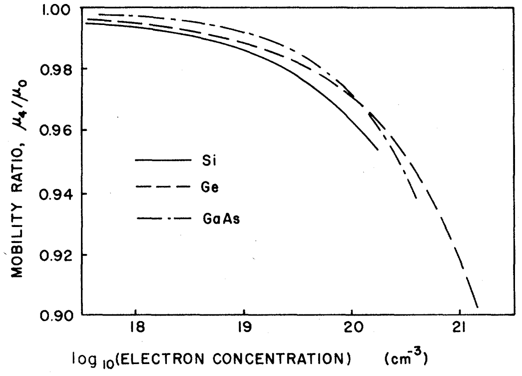

FIG. 6. Ratio of electron mobilities, μ_4/μ_0, for silicon, germanium, and gallium arsenide at $T = 300$ K as a function of electron concentration.

ACKNOWLEDGMENTS

The authors are grateful to the University of Vermont for making available the resources of its academic computing center. Thanks also go to W. P. Rogers for computational assistance.

---

[1] H. Brooks, Phys. Rev. 83, 879 (1951); *Advances in Electronics and Electron Physics*, edited by L. Marton (Academic, New York, 1955), Vol. 7, p. 128; C. Herring (unpublished). The actual derivation and requisite assumptions of the BH theory have been given by L. M. Falicov and M. Cuevas, Phys. Rev. 164, 1025 (1967). R. B. Dingle, Philos. Mag. 46, 831 (1955), and R. Mansfield, Proc. Phys. Soc. (London) B69, 76 (1956) introduce a form of the BH theory which deals with arbitrary carrier degeneracy and assumes that all impurities are ionized. Refer also to R. Barrie, Proc. Phys. Soc. (London) B69, 553 (1956) for similar considerations.

[2] E. Conwell and V. F. Weisskopf, Phys. Rev. 69, 258 (1946); 77, 388 (1950). An extension of the CW theory to the case of a degenerate electron gas has been developed by V. A. Johnson and K. Lark-Horowitz, Phys. Rev. 71, 374 (1947).

[3] N. F. Mott, Proc. Cambridge Philos. Soc. 32, 281 (1936), included space charge screening of ionized-impurity centers in a way suitable for impure metals. This treatment obtains only for the Thomas-Fermi model of degenerate electron systems.

[4] The screened Coulomb potential appears in the theory of electrolytes originally formulated by P. Debye and E. Hückel, Z. Phys. 24, 185, 305 (1923).

[5] A straightforward bridging between the screening and nonscreening situations of the BH and CW theories is possible if a consistent one-center-scattering approximation is adopted. Refer to B. K. Ridley, J. Phys. C 10, 1589 (1977).

[6] P. P. Debye and E. M. Conwell, Phys. Rev. 93, 693 (1954).

[7] L. M. Richardson and L. M. Scarfone, Phys. Rev. B 19, 5139 (1979).

[8] A preliminary report of this work appeared in the Bull. Am. Phys. Soc. 24, 762 (1979).

[9] The first impurity-ion potential devised by P. Csavinszky, Phys. Rev. B 14, 1649 (1976), as an approximate solution of the linearized Poisson equation, with the neglect of the term involving $\kappa'(r)$, behaves improperly at the origin. A subsequent investigation by the same author, Int. J. Quantum Chem. 13, 221 (1978), outlines how this defect in the potential at small radial distances can be eliminated, and the corrected ion potential is given.

[10] M. Azuma and K. Shindo, J. Phys. Soc. Jpn. 19, 424 (1964). There appear to be two misprints in this reference. See first citation in Ref. 9, Footnote 8, for details.

[11] J. Okuro and M. Azuma, J. Phys. Soc. Jpn. 20, 1099 (1964).

[12] D. R. Penn, Phys. Rev. 128, 2093 (1962). Besides this original work there is also the effort by G. Srin-

ivasan, *ibid.* 178, 1244 (1969), who reconsiders Penn's model in detail and obtains consistent expressions for the wave-vector-dependent dielectric function over the entire range of the wave vector. These results agree fairly well with those of J. P. Walter and M. L. Cohen, Phys. Rev. B 2, 1821 (1970); 5, 3101 (1972), who use the accurate pseudopotential random-phase approximation method to evaluate the longitudinal wave-vector-dependent dielectric function for several elemental and compound semiconductors. Refer also to H. Nara, J. Phys. Soc. Jpn. 20, 778, 1097 (1965); P. K. Vinsome and M. Jaros, J. Phys. C 3, 2140 (1970); 4, 1360 (1971); P. K. Vinsome and D. Richardson, *ibid.* 4, 2650 (1971).

[13] Several authors [L. M. Richardson and L. M. Scarfone, Bull. Am. Phys. Soc. 23, 115 (1978); M. A. Paesler, Phys. Rev. B 17, 2059 (1978); L. M. Richardson and L. M. Scarfone, *ibid.* 18, 5892 (1978); M. A. Paesler, P. E. Theodorou, and H. J. Queisser, *ibid.* 18, 5895 (1978); D. E. Theodorou and H. J. Queisser, *ibid.* 18, 2092 (1979)] have provided comparisons between the mobility calculated with ϕ_1, and the Dingle mobility. The disagreement between the conclusions in the second and third of the above citations is due to a mathematical error in the former. The absence of this error in the fourth and fifth citations leads to results for the mobility which are in agreement with those of Richardson and Scarfone for low carrier concentrations and somewhat different in the heavily doped regime.

[14] L. M. Richardson and L. M. Scarfone, Phys. Rev. B 19, 925 (1979).

[15] K. R. Brownstein, Phys. Rev. B 15, 5073 (1977); P. Csavinszky, *ibid.* 17, 2793 (1978); K. R. Brownstein, *ibid.* 17, 2795 (1978).

[16] R. Resta, Phys. Rev. B 16, 2717 (1977); F. Cornolti and R. Resta, *ibid.* 17, 3239 (1978).

[17] H. Nara and A. Morita, J. Phys. Soc. Jpn. 21, 1852 (1966); K. R. Schulze and K. Unger, Phys. Status Solidi B 66, 491 (1974). Consult also the first two citations in Ref. 12.

[18] R. Resta, Phys. Rev. B 19, 3022 (1979). A comparison between the ion-impurity potential developed in Ref. F and that based on Eq. (9) for $R_0=30$ a.u. shows that, while both potentials are stronger than ϕ_0 only at small r, the former is stronger than the latter. See also Richard A. Morrow, Phys. Rev. B 21, 1698 (1980). This work shows the approximate equivalence of the Csavinszky and Resta models of impurity-ion potentials in semiconductors.

[19] R. Beckett and J. Hurt, *Numerical Calculations and Algorithms*, (McGraw-Hill, New York, 1967).

[20] The approximation entails letting $\kappa(r)$ become κ_0 at a certain point in the variational calculation. Details may be found in Appendix Y of L. M. Richardson's doctoral thesis submitted to the University of Vermont in 1979 (unpublished). Copies available from University Microfilms, Ann Arbor, Michigan.

[21] J. Blakemore, *Semiconductor Statistics*, (Pergamon, Oxford, 1962).

[22] P. Csavinszky, Phys. Rev. B 17, 3177 (1978).

[23] J. R. Meyer, Phys. Rev. B 20, 1762 (1979).