

Theory of the screening of impurity ions in semiconductors with spatially-variable dielectric constants*

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In this paper, Dingle's theory of the screening of impurity ions in semiconductors is generalized. This is accomplished by inserting in the theory of screening the spatial dielectric function of the medium. Poisson's equation for the potential of an impurity ion follows from one of Maxwell's equations. With the analytical form for the spatial dielectric function for Si and Ge, obtained for these materials by Azuma and Shindo and by Okuro and Azuma, Poisson's equation assumes a specific form. The asymptotic form of this differential equation, the region where the theory is expected to be valid, is solved approximately by an equivalent variational principle. The end result of the present theory is an impurity-ion potential which is represented by a linear combination of two exponentially screened Coulomb potentials scaled by the static dielectric constant of the medium. Each of the screening lengths appearing in the screened Coulomb potentials is related to Dingle's screening length. Numerical data, as functions of charge carrier concentration, are given both for the screening lengths, and for the coefficients involved in the linear combination of the two screened Coulomb potentials. It is concluded that the form obtained in the present paper for the potential of an impurity ion leads to modifications in theories of ionized-impurity scattering in semiconductors.

I. INTRODUCTION

One of the important scattering processes, on which charge transport in doped semiconductors depends, is the scattering of charge carriers by ionized impurity atoms.

Theoretical treatments of this scattering process, such as the well-known theories of Conwell and Weisskopf,¹ of Brooks and Herring,² or the less often used partial-wave theories of Blatt,³ of Csavinszky,⁴ and of Krieger and Strauss,⁵ are all based on the choice of a potential that an impurity ion in a semiconductor is assumed to have.

A comprehensive treatment of the screening of charged (point) impurity atoms in semiconductors with spherical energy surfaces has been given by Dingle.⁶ In his theory, a particular semiconductor is accounted for by a given (isotropic) effective mass of the charge carrier, and by a given static dielectric constant. The end result of Dingle's theory is an exponentially screened Coulomb potential for an impurity ion, which is scaled by the static dielectric constant of the medium. This potential is obtained by solving Poisson's equation, which connects the potential of the impurity ion with the charge density of its screening cloud which, itself, is composed of free charge carriers in their respective bands.

The purpose of the present paper is the generalization of Dingle's theory. This is attempted by replacing the static dielectric constant in the Poisson's equation of Dingle by the spatial dielectric function of the medium. This step, as shown in the Appendix, is equivalent to solving the asymptotic form of Poisson's equation for the potential of an impurity ion in a medium which is characterized by a spatially-variable dielectric constant

of a specific analytical form. The analytical approximations to the spatial dielectric function considered in this paper has been obtained, on the basis of the Penn⁷ model, by Azuma and Shindo⁸ for Si, and by Okuro and Azuma⁹ for Ge.¹⁰ The differential equation describing the asymptotic form of Poisson's equation is more complicated than that encountered in Dingle's theory. It is solved approximately by making use of an equivalent variational principle. The end result of the present theory is an impurity-ion potential which is represented by a linear combination of two exponentially screened Coulomb potentials scaled by the static dielectric constant of the medium. Each of the screening lengths appearing in the screened Coulomb potentials is different from, but related to the screening length of Dingle. Numerical values, as a function of the concentration of free charge carriers, are given both for each of the screening lengths, and for the coefficients involved in the linear combination of the two screened Coulomb potentials. The form obtained in the present paper for the potential of an impurity ion is expected to lead to fairly obvious modifications of both the Brooks-Herring theory, and of the partial wave theories of ionized-impurity scattering.

The paper is structured as follows. In Sec. II the modified impurity ion potential is derived. In Sec. III the potential obtained is compared with the potential of Dingle. In Sec. IV the dielectric function is discussed. In Sec. V some concluding comments are advanced.

II. THEORY

For the sake of simplicity, we shall consider an *n*-type (uncompensated) impurity semiconductor

in which one excess electron is provided by each donor atom, which, therefore, becomes a singly charged positive ion.

To establish our notation, we shall first rederive Dingle's result for the potential of a donor ion, and then we shall proceed with the modifications.

Let ν represent the number of electrons per unit volume in the conduction band resulting from the ionization of the donors, and let φ represent the electrostatic potential of a donor ion. Then the Fermi energy, ζ_ν , must be replaced by $\zeta_\nu + e_0\varphi(r)$, where e_0 is the magnitude of the electron charge.

The number of electrons per unit volume near a donor ion is given by

$$\nu(r) = \frac{8\pi\sqrt{2} m^{*3/2}}{h^3} \times \int_0^\infty \frac{E^{1/2} dE}{\exp\{[E - \zeta_\nu - e_0\varphi(r)]/k_B T\} + 1}, \quad (1)$$

where, assuming the energy band to be quadratic, m^* is an isotropic effective electron mass, while the other quantities have their conventional meaning.

Introducing the Fermi-Dirac integrals by

$$\mathcal{F}_k(\eta) = \frac{1}{k!} \int_0^\infty \frac{x^k dx}{e^{(x-\eta)} + 1}, \quad (2)$$

we can rewrite Eq. (1) as

$$\nu(r) = \frac{4\pi(2\pi)^{1/2} m^{*3/2} (k_B T)^{3/2}}{h^3} \times \mathcal{F}_{1/2}\left(\eta_\nu + \frac{e_0\varphi(r)}{k_B T}\right), \quad (3)$$

where the reduced Fermi level is defined by

$$\eta_\nu = \zeta_\nu / k_B T. \quad (4)$$

At large values of r , where $\varphi(r)$ is expected to be small, the function $\mathcal{F}_{1/2}$ can be expanded in terms of $e_0\varphi(r)/k_B T$. Defining the screening charge by

$$\rho(r) = e_0[\nu - \nu(r)], \quad (5)$$

where ν is given by Eq. (1) with $\varphi(r) = 0$, and making use of the relation

$$\mathcal{F}'_k(\eta) = \mathcal{F}_{k-1}(\eta), \quad (6)$$

the expansion of Eq. (3), upon consideration of Eq. (5), gives for the space dependence of the screening charge

$$\rho(r) = -\frac{4\pi e_0^2 m^{*3/2} (2k_B T)^{1/2}}{h^3} \mathcal{F}_{-1/2}(\eta_\nu) \varphi(r). \quad (7)$$

With this form for $\rho(r)$, we wish to obtain $\varphi(r)$ as a solution of Poisson's equation, given by

$$\nabla^2 \varphi(r) = -\frac{4\pi\rho(r)}{\kappa_0}, \quad (8)$$

where κ_0 is the static dielectric constant of the medium. We shall refer to Eq. (8) as the unmodified Poisson's equation.

Introducing the notation

$$R_0^{-2} = \frac{16\pi^2 e_0^2 m^{*3/2} (2\pi k_B T)^{1/2}}{\kappa_0 h^3} \mathcal{F}_{-1/2}(\eta_\nu), \quad (9)$$

where R_0 , as will be seen later, is the Dingle screening length, Eq. (8) can be expressed as

$$\varphi'' + (2/r)\varphi' - R_0^2 \varphi = 0. \quad (10)$$

Equation (10) is to be solved with the boundary conditions

$$\varphi(r \rightarrow 0) = e_0/\kappa_0 r \quad (11)$$

and

$$\varphi(r \rightarrow \infty) = 0. \quad (12)$$

The general solution of Eq. (10) is

$$\varphi(r) = k_1(e^{-r/R_0}/r) + k_2(e^{+r/R_0}/r), \quad (13)$$

where the constants k_1 and k_2 are determined by imposing the boundary conditions on $\varphi(r)$ in Eq. (13).

The boundary condition in Eq. (12) requires that $k_2 = 0$, while the boundary condition in Eq. (11) demands that $k_1 = e_0/\kappa_0$. Thus Eq. (13) reduces to

$$\varphi(r) = (e_0/\kappa_0 r) e^{-r/R_0}, \quad (14)$$

which is the Dingle potential of a donor ion.

It should be mentioned here in passing that attempts have been made to improve on the potential in Eq. (14) by considering higher-order terms in the expansion of $\mathcal{F}_{1/2}$ in Eq. (3). Csavinszky¹¹ has considered the effect of the second-order term, and Adawi¹² has further generalized the theory to all orders. The resulting nonlinear differential equations, however, lead to quite complicated correction terms to Eq. (14) and, to the author's knowledge, has so far not been used in theories of ionized impurity scattering.

Our proposed modification of Dingle's theory consists in the replacement of κ_0 in Eq. (8) by the spatial dielectric function $\kappa(r)$ of the medium. This step carries with it two assumptions. First, it is assumed that the spherically symmetric but not pointlike screening charge, which is made up of free electrons in the conduction band, is itself screened by the electrons participating in the binding of the crystal in the same way as a point charge is screened by them. Second, it is assumed that the dielectric function in a doped semiconductor can be taken to be the same as that in the pure crystal.

The analytical approximation of the spatial dielectric function, obtained on the basis of the Penn⁷ model by Azuma and Shindo⁸ for Si, and by Okuro and Azuma⁹ for Ge, is of the form

TABLE I. Parameters in the spatial dielectric function.

Semiconductor	A	B	$\frac{\alpha}{(a_B^{-1})}$	$\frac{\beta}{(a_B^{-1})}$	$\frac{\gamma}{(a_B^{-1})}$
Ge	0.0544	0.0080	0.9668	0.3757	0.7460
Si	0.0726	0.0107	0.663	0.9129	0.302

$$\kappa(r)^{-1} = e^{-\alpha r} + A(1 - e^{-\beta r}) + B(1 - e^{-\gamma r}), \quad (15)$$

where the constants appearing in Eq. (7) are given in Table I.¹³

Considering that according to Eq. (15), at large values of r , we have

$$1/\kappa(\infty) = A + B = 1/\kappa_0, \quad (16)$$

we can rewrite Eq. (8) as

$$\nabla^2 \phi(r) = -\frac{4\pi\rho(r)}{\kappa_0} - 4\pi\rho(r)(e^{-\alpha r} - A e^{-\beta r} - B e^{-\gamma r}), \quad (17)$$

where ϕ has been written for the previous φ .

It is mentioned here that $(A+B)^{-1}$ is not exactly equal to the experimental value for κ_0 . Using the data in Table I, we have $\kappa_0 = 16.03$ for Ge, and $\kappa_0 = 12.00$ for Si, while the experimental values for Ge and Si, as given by Dunlap and Watters,¹⁴ are 15.8 and 11.7, respectively. For the sake of consistency, we shall, however, use $(A+B)^{-1}$ for κ_0 .

With the aid of Eqs. (7) and (9), an alternative form for Eq. (17) is

$$\phi'' + \frac{2}{r}\phi' - R_0^{-2}\phi = \kappa_0 R_0^{-2}\phi(e^{-\alpha r} - A e^{-\beta r} - B e^{-\gamma r}). \quad (18)$$

We shall call Eq. (18) the modified Poisson's equation, in contrast to Eq. (10) which we have called the unmodified Poisson's equation. It is seen from Eq. (18) that the modified Poisson's equation is still a homogeneous differential equation since it can also be written in the form

$$\phi'' - (2/r)\phi' - R_0^{-2}[1 + \kappa_0(e^{-\alpha r} - A e^{-\beta r} - B e^{-\gamma r})]\phi = 0. \quad (18a)$$

It is also seen from Eq. (18a) that the term in square parentheses is a correction term, a sort of a "perturbation," which becomes small with increasing r . It is, therefore, reasonable to assume that the overall features of the donor-ion problem are accounted for by the Dingle model. For this reason we are going to seek the solution of the modified Poisson's equation with the boundary conditions of Dingle.⁶

To proceed further, the transformation

$$\psi = r\phi \quad (19)$$

is introduced. In terms of ψ , the differential equation in Eq. (18) assumes the simpler form

$$\psi'' - R_0^{-2}\psi = \kappa_0 R_0^{-2}\psi(e^{-\alpha r} - A e^{-\beta r} - B e^{-\gamma r}), \quad (20)$$

which is to be solved with the boundary conditions

$$\psi(0) = 1 \quad (21)$$

and

$$\psi(\infty) = 0, \quad (22)$$

as follows from Eqs. (11) and (12) upon consideration of Eq. (19). It should be noted here, however, that Eq. (21) has been written without the e_0/κ_0 factor. This is permissible in view of the fact that Eq. (18a) is a homogeneous differential equation (e_0/κ_0 is introduced in the end result).

We propose to obtain an approximate solution of Eq. (20) by making use of an equivalent variational principle. This is a procedure which often can be used to advantage in mathematical physics.¹⁵

Let us consider the functional

$$I[\psi] = \int_0^\infty F(\psi, \psi', r) dr, \quad (23)$$

where ψ' stands for the derivative of ψ with respect to r . Let us now choose F as

$$F = -\frac{1}{2}(\psi')^2 - \frac{1}{2}R_0^{-2}\psi^2 - \frac{1}{2}\kappa_0 R_0^{-2}e^{-\alpha r}\psi^2 + \frac{1}{2}\kappa_0 R_0^{-2}A e^{-\beta r}\psi^2 + \frac{1}{2}\kappa_0 R_0^{-2}B e^{-\gamma r}\psi^2, \quad (24)$$

where ψ is an appropriately chosen function that depends on several parameters.

The expression for F , in Eq. (24), is such that upon its substitution into the Euler-Lagrange equation, given by¹⁶

$$\frac{\partial}{\partial \psi} F - \frac{\partial}{\partial r} \frac{\partial}{\partial \psi'} F = 0, \quad (25)$$

the modified Poisson's equation as given by Eq. (20) results. With a given choice for ψ , one then proceeds by extremalizing I in Eq. (23) with respect to the parameters in ψ . By this procedure one thus obtains an approximate solution of Eq. (20).

There remains the making of a judicious choice for ψ . This is dictated, upon consideration of the boundary conditions in Eqs. (21) and (22), chiefly by expediency. Let us say that, if possible, it would be advantageous to represent ψ as a linear combination of exponentials. In this case, the formulas worked out in theories of ionized impurity scattering on the basis of the Dingle potential could be utilized with the potential proposed. The appropriate modifications required would only be of a simple nature.

In the light of what was just said, we assume the following form for ψ :

$$\psi = C e^{-(a-b)r} + D e^{-(a+b)r}, \quad (26)$$

where C , D , a , and b are parameters to be determined.

For our solution to be meaningful, we must have

$$a - b > 0 \tag{27} \quad D = 1 - C, \tag{29}$$

and

$$a + b > 0, \tag{28}$$

as required by the boundary condition in Eq. (22).

Imposing the boundary condition in Eq. (21) on ψ , as given in Eq. (26), we obtain

so that instead of four, we are now left only with three independent parameters.

Using Eq. (26), and forming $\psi' = d\psi/dr$, we can build Eq. (24) and evaluate the integral in Eq. (23). The result can be expressed as

$$I = -\frac{1}{2} \left[\left(C^2 \frac{a-b}{2} + (C-C^2) \frac{a^2-b^2}{a} + (1-C)^2 \frac{a+b}{2} \right) + R_0^2 \left(C^2 \frac{1}{2(a-b)} + (C-C^2) \frac{1}{a} + (1-C)^2 \frac{1}{2(a+b)} \right) \right. \\ \left. + \kappa_0 R_0^{-2} \left(C^2 \frac{1}{2a-2b+\alpha} + (C-C^2) \frac{2}{2a+\alpha} + (1-C)^2 \frac{1}{2a+2b+\alpha} \right) - \kappa_0 R_0^{-2} A \left(C^2 \frac{1}{2a-2b+\beta} + (C-C^2) \frac{2}{2a+\beta} \right. \right. \\ \left. \left. + (1-C)^2 \frac{1}{2a+2b+\beta} \right) - \kappa_0 R_0^{-2} B \left(C^2 \frac{1}{2a-2b+\gamma} + (C-C^2) \frac{2}{2a+\gamma} + (1-C)^2 \frac{1}{2a+2b+\gamma} \right) \right]. \tag{30}$$

We shall now consider the parameter a as a fixed quantity. The reason for this will be discussed later. This leaves us only with two parameters, b and C , which are determined from the requirements

$$\frac{\partial I[\psi]}{\partial C} = 0 \tag{31}$$

and

$$\frac{\partial I[\psi]}{\partial a} = 0. \tag{32}$$

Carrying out the differentiation in Eq. (31), we find, after some algebra, that the result can be expressed as

$$-b - \frac{b^2}{a} + R_0^{-2} \frac{b}{a(a+b)} + 2\kappa_0 R_0^{-2} \left(\frac{1}{2a+\alpha} - \frac{1}{2a+2b+\alpha} \right) - 2\kappa_0 R_0^{-2} A \left(\frac{1}{2a+\beta} - \frac{1}{2a+2b+\beta} \right) - 2\kappa_0 R_0^{-2} B \left(\frac{1}{2a+\gamma} - \frac{1}{2a+2b+\gamma} \right) \\ + C \left[\frac{2b^2}{a} + R_0^{-2} \left(\frac{1}{a-b} + \frac{1}{a+b} - \frac{2}{a} \right) + 2\kappa_0 R_0^{-2} \left(\frac{1}{2a-2b+\alpha} + \frac{1}{2a+2b+\alpha} - \frac{2}{2a+\alpha} \right) \right. \\ \left. - 2\kappa_0 R_0^{-2} A \left(\frac{1}{2a-2b+\beta} + \frac{1}{2a+2b+\beta} - \frac{2}{2a+\beta} \right) - 2\kappa_0 R_0^{-2} B \left(\frac{1}{2a-2b+\gamma} + \frac{1}{2a+2b+\gamma} - \frac{2}{2a+\gamma} \right) \right] = 0. \tag{33}$$

Similarly, we find that Eq. (32) results in the expression

$$-\frac{1}{2} C^2 - \frac{2b}{a} (C-C^2) + \frac{1}{2} (1-C)^2 + \frac{1}{2} R_0^{-2} \left(C^2 \frac{1}{(a-b)^2} - (1-C)^2 \frac{1}{(a+b)^2} \right) + 2\kappa_0 R_0^{-2} \left(C^2 \frac{1}{(2a-2b+\alpha)^2} \right. \\ \left. - (1-C)^2 \frac{1}{(2a+2b+\alpha)^2} \right) - 2\kappa_0 R_0^{-2} A \left(C^2 \frac{1}{(2a-2b+\beta)^2} - (1-C)^2 \frac{1}{(2a+2b+\beta)^2} \right) - 2\kappa_0 R_0^{-2} B \left(C^2 \frac{1}{(2a-2b+\gamma)^2} \right. \\ \left. - (1-C)^2 \frac{1}{(2a+2b+\gamma)^2} \right) = 0. \tag{34}$$

Let us now make the assumption that

$$a = R_0^{-1} \tag{35}$$

and

$$b = nR_0^{-1}, \tag{36}$$

where n is now our new parameter taking the place of b . With this assumption, we have changed the independent parameters from (b, C) to (n, C) .

To satisfy the requirements in Eqs. (27) and (28), n must be such that

$$1 - n > 0 \tag{37}$$

and

$$1 + n > 0. \tag{38}$$

Equations (37) and (38) permit n to be either positive, or negative, with values restricted to the interval

$$-1 < n < 1. \tag{39}$$

With the choices made for a and b in Eqs. (35) and (36), we see that

$$a - b = (1 - n)R_0^{-1} \tag{40}$$

and

TABLE II. Parameters entering into the potential of a donor ion in Ge as functions of the Dingle screening length.

R_0 (a_B)	$-n$	C
15	0.3988	0.7060
20	0.3087	0.6580
25	0.2512	0.6278
30	0.2115	0.6072
35	0.1825	0.5922
40	0.1605	0.5809
45	0.1431	0.5721
50	0.1291	0.5650
55	0.1176	0.5591
60	0.1080	0.5543
65	0.0998	0.5501
70	0.0928	0.5466
75	0.0867	0.5435
80	0.0813	0.5408
85	0.0766	0.5384
90	0.0724	0.5363
95	0.0686	0.5344
100	0.0652	0.5327
105	0.0621	0.5311
110	0.0593	0.5297
115	0.0567	0.5284
120	0.0544	0.5272
125	0.0522	0.5262
130	0.0502	0.5251
135	0.0484	0.5242
140	0.0467	0.5234
145	0.0451	0.5226
150	0.0436	0.5218
155	0.0422	0.5211
160	0.0409	0.5204
165	0.0396	0.5198
170	0.0385	0.5192
175	0.0374	0.5187
180	0.0363	0.5182
185	0.0354	0.5177
190	0.0344	0.5172
195	0.0335	0.5168
200	0.0327	0.5164
205	0.0319	0.5160
210	0.0312	0.5156
215	0.0305	0.5152
220	0.0298	0.5149
225	0.0291	0.5146
230	0.0284	0.5142
235	0.0278	0.5139
240	0.0273	0.5136
300	0.0218	0.5109
400	0.0164	0.5082
500	0.0132	0.5065
600	0.0110	0.5055
700	0.0096	0.5047
800	0.0083	0.5041
900	0.0075	0.5036
1000	0.0068	0.5033
2000	0.0046	0.5017
3000	0.0038	0.5013
4000	0.0037	0.5011
5000	0.0035	0.5010

$$a + b = (1 + n)R_0^{-1}. \quad (41)$$

Using Eqs. (40) and (41), we can rewrite Eq. (26) as

$$\psi = C e^{-(1-n)(r/R_0)} + D e^{-(1+n)(r/R_0)}, \quad (42)$$

so that the quantities

$$R_1 = R_0/(1 - n) \quad (43)$$

and

$$R_2 = R_0/(1 + n), \quad (44)$$

play the role of screening lengths.

Substitution of Eqs. (35) and (36) into Eq. (33) leads to an expression for C . We find, after some algebra, that

$$C = \frac{Q_1 - 2\kappa_0(L_\alpha - AL_\beta - BL_\gamma)}{Q_2 + 2\kappa_0(K_\alpha - AK_\beta - BK_\gamma)}, \quad (45)$$

where

$$Q_1 = \frac{2n^2 + n^3}{1 + n}, \quad (46)$$

$$Q_2 = \frac{4n^2 - 2n^4}{1 - n^2}, \quad (47)$$

and, using the notation $q = \alpha, \beta, \gamma$, the other quantities are defined by

$$L_q = \frac{1}{2}O_q - N_q^{1/2}, \quad (48)$$

$$K_q = M_q^{1/2} + N_q^{1/2} - O_q, \quad (49)$$

with

$$M_q = (2 - 2n + qR_0)^{-2}, \quad (50)$$

$$N_q = (2 + 2n + qR_0)^{-2}, \quad (51)$$

$$O_q = 2(2 + qR_0)^{-2}. \quad (52)$$

Similarly, we find that Eq. (34) can be brought to the form

$$\begin{aligned} & -\frac{1}{2}[C^2 + 4nC(1 - C) - (1 - C)^2] + \frac{1}{2}[C^2(1 - n)^{-2} \\ & - (1 - C)^2(1 + n)^{-2}] + 2\kappa_0[C^2M_\alpha - (1 - C)^2N_\alpha] \\ & - 2\kappa_0A[C^2M_\beta - (1 - C)^2N_\beta] \\ & - 2\kappa_0B[C^2M_\gamma - (1 - C)^2N_\gamma] = 0. \end{aligned} \quad (53)$$

Substituting the expression for C from Eq. (45) into Eq. (53), the task is the finding of that value of n which, for a given choice of R_0 , makes the left-hand side of Eq. (53) equal to zero.

Values of n and C , calculated for a wide range of the Dingle screening length R_0 , are given for Ge in Table II, and for Si in Table III.

Considering Eqs. (19), (26), and (29), our donor-ion potential, in terms of C , n , and R_0 , is expressed (with the e_0/κ_0 factor) as

$$\phi(r) = (e_0/\kappa_0 r) [C e^{-r/R_1} + (1 - C) e^{-r/R_2}], \quad (54)$$

where R_1 and R_2 are defined by Eqs. (43) and (44).

TABLE III. Parameters entering into the potential of a donor ion in Si as functions of the Dingle screening length.

R_0 (a_B)	$-n$	C
15	0.5068	0.7709
20	0.4056	0.7149
25	0.3378	0.6775
30	0.2892	0.6510
35	0.2528	0.6313
40	0.2245	0.6161
45	0.2018	0.6040
50	0.1833	0.5942
55	0.1679	0.5861
60	0.1549	0.5793
65	0.1438	0.5734
70	0.1341	0.5684
75	0.1257	0.5640
80	0.1182	0.5602
85	0.1116	0.5567
90	0.1057	0.5537
95	0.1004	0.5509
100	0.0956	0.5485
105	0.0912	0.5462
110	0.0872	0.5442
115	0.0836	0.5423
120	0.0802	0.5406
125	0.0771	0.5390
130	0.0742	0.5375
135	0.0716	0.5362
140	0.0691	0.5349
145	0.0668	0.5337
150	0.0646	0.5326
155	0.0626	0.5316
160	0.0607	0.5306
165	0.0589	0.5297
170	0.0572	0.5288
175	0.0556	0.5280
180	0.0541	0.5273
185	0.0527	0.5265
190	0.0513	0.5258
195	0.0500	0.5252
200	0.0488	0.5246
205	0.0477	0.5240
210	0.0465	0.5234
215	0.0455	0.5229
220	0.0445	0.5224
225	0.0435	0.5219
230	0.0426	0.5214
235	0.0417	0.5210
240	0.0408	0.5205
300	0.0328	0.5165
400	0.0247	0.5124
500	0.0197	0.5099
600	0.0165	0.5083
700	0.0143	0.5071
800	0.0124	0.5062
900	0.0110	0.5055
1000	0.0100	0.5052
2000	0.0056	0.5025
3000	0.0041	0.5017
4000	0.0037	0.5013
5000	0.0032	0.5011

Equation (54), together with Eqs. (43) and (44), represent the central result of this paper. They constitute an approximate solution of the modified Poisson's equation which is given by Eq. (18). The dependence of ϕ on m^* , κ_0 , and on the electron concentration ν , via the reduced Fermi level η_ν , is contained in R_0 . For the last-mentioned quantity several simple limiting forms can be given.

For a highly degenerate electron gas $\eta_\nu \gg 0$, and application of the asymptotic relation⁶

$$\mathcal{F}_k(\eta) \sim \eta^{k+1}/(k+1)! \quad (55)$$

permits us to obtain from Eq. (9) the limiting form

$$R_{0,d} = \left(\frac{\pi}{3}\right)^{1/6} \frac{\hbar \kappa_0^{1/2}}{4\pi e_0 m_0^{1/2}} \delta^{-1/2} \nu^{-1/6}, \quad (56)$$

where $\delta = m^*/m_0$ is the ratio of the effective electron mass to the real electron mass.

For a highly nondegenerate electron gas $\eta_\nu \ll 0$, and application of the approximation⁶

$$\mathcal{F}_k(\eta) \approx e^\eta \quad (57)$$

permits us to deduce from Eq. (9) the limiting form

$$R_{0,n} = (\kappa_0 k_B T)^{1/2} / (4\pi \nu)^{1/2} e_0. \quad (58)$$

The formula in Eq. (56) is valid when $T < T_d$, while that in Eq. (58) is valid when $T > T_d$, where the degeneracy temperature is defined by

$$T_d = \frac{\hbar^2}{8m_0 k_B} \left(\frac{3}{\pi}\right)^{2/3} \nu^{2/3} \delta^{-1}. \quad (59)$$

For intermediate degeneracy, where $T \approx T_d$, the full expression for R_0 , as given in Eq. (9), has to be used. Extensive tables of Fermi-Dirac integrals, defined by

$$F_k(\eta) = k! \mathcal{F}_k(\eta), \quad (60)$$

are given by McDougall and Stoner.¹⁷

It is seen from Tables II and III that, at large values of R_0 , we have $|n| \rightarrow 0$, and $C \rightarrow \frac{1}{2}$. In this limit, therefore, the modified donor ion potential, given in Eq. (54), goes over into Dingle's potential, given in Eq. (14). Inspection of Eq. (58) shows that, at a fixed T , large values of R_0 are associated with a nondegenerate electron gas, i. e., with low electron concentrations. It is also seen from Tables I and II that larger values of $|n|$ occur at smaller values of R_0 which range, upon inspection of Eq. (56), is associated with a degenerate electron gas.¹⁸

III. MODIFIED POTENTIAL

For theories of ionized impurity scattering it is of great interest to compare Dingle's potential with our modified potential of a donor ion. An investigation of the ratio

TABLE IV. Ratio of the potential obtained in this paper to that of Dingle for Ge.

r	$f(r)$		
	$R_0 = 30 a_B$	$R_0 = 60 a_B$	$R_0 = 90 a_B$
0	1.000	1.000	1.000
10	1.012	1.002	1.001
20	1.021	1.003	1.001
30	1.024	1.004	1.001
40	1.022	1.005	1.002
50	1.015	1.006	1.002
60	1.003	1.006	1.002
70	0.986	1.006	1.003
80	0.965	1.005	1.003
90	0.941	1.005	1.003
100	0.913	1.003	1.003
120	0.850	1.000	1.002
140	0.781	0.996	1.002
160	0.709	0.990	1.001
180	0.638	0.983	1.000
200	0.569	0.975	0.999
300	0.300	0.919	0.989
400	0.151	0.844	0.972
500	0.075	0.757	0.951
600	0.037	0.666	0.924
700	0.018	0.579	0.893
800	0.009	0.497	0.859
900	0.004	0.423	0.822
1000	0.002	0.359	0.784

$$f(r) = \frac{e^{-r/R_0}}{C e^{-r/R_1} + (1-C) e^{-r/R_2}} \quad (61)$$

may give us some insight into the importance of replacing in Poisson's equation the static dielectric constant by the spatial dielectric function of the medium.

Before we embark on obtaining $f(r)$ from Eq. (61), a comment on the parameter n is in order. In performing the present work, the numerical calculations of n and C have first been carried out in the $-1 < n < 0$ range. Subsequent calculations in the $0 < n < 1$ range have, however, shown that $\partial I / \partial b$ is symmetric with respect to its zeros. This means that C as a function of $-n$ is equal to $(1-C)$ as a function of $+n$. To avoid confusing tabulations, we have only listed, in Tables II and III, the C values which go with $-n$.

Values of $f(r)$, as a function of r , for several values of R_0 , are shown in Table IV for Ge, and in Table V for Si. It is seen from these tables that, for smaller values of R_0 , the potential ratio $f(r)$ becomes smaller than unity for moderate values of r . The larger is R_0 , the farther away one must go from the donor ion to have $f(r)$ appreciably less than one. From the inspection of the data we must, therefore, conclude that in the case of a degenerate electron gas, corresponding to heavy doping, the present modification of the

Dingle potential is more important than in the case of a nondegenerate electron gas, that corresponds to light doping.

IV. DIELECTRIC FUNCTION

The wave-vector-dependent dielectric function describes the static screening of a longitudinal electric field which varies in space. In other words, this quantity describes the crystal response to an electric field parallel to the wave vector. For this reason, the dielectric function is sometimes also referred to as the response function. If the electric field results from placing a charge in a medium, then the charge will have its field altered by the medium which tends to shield the charge. This shielding effect is described by the dielectric function. The chief contribution to the shielding of a point charge in an undoped semiconductor crystal results from the electrons participating in the chemical bonds. The dielectric function, at large distances from the charge, assumes the value of the static dielectric constant of the medium. For this reason, we can also talk of a spatially-variable dielectric constant even though this usage appears to be somewhat confusing unless we are prepared to look at this quantity in the enlarged sense of considering it a constant at a given distance from the charge.

Penn,⁷ on the basis of a formula given by Ehren-

TABLE V. Ratio of the potential obtained in this paper to that of Dingle for Si.

r	$f(r)$		
	$R_0 = 30 a_B$	$R_0 = 60 a_B$	$R_0 = 90 a_B$
0	1.000	1.000	1.000
10	1.025	1.004	1.001
20	1.042	1.007	1.002
30	1.049	1.009	1.003
40	1.046	1.011	1.004
50	1.034	1.012	1.005
60	1.013	1.013	1.005
70	0.983	1.013	1.005
80	0.947	1.012	1.006
90	0.905	1.011	1.006
100	0.860	1.008	1.006
120	0.761	1.002	1.005
140	0.660	0.993	1.004
160	0.565	0.982	1.003
180	0.478	0.968	1.000
200	0.401	0.952	0.998
300	0.158	0.848	0.976
400	0.061	0.721	0.943
500	0.023	0.592	0.900
600	0.009	0.475	0.850
700	0.003	0.376	0.794
800	0.001	0.295	0.736
900	0.000	0.230	0.677
1000	0.000	0.178	0.619

reich and Cohen,¹⁹ has discussed a crude approximation to the dielectric function. In this approximation, if the static dielectric constant is much greater than unity, then the dielectric function can be approximated by its value for the free electron gas. An analytic expression for this quantity for the case of a free electron gas has been derived by Hubbard.²⁰

A more refined approximation for the dielectric function of a semiconductor has been given by Callaway,²¹ who introduced the energy gap into the model. In his model, the semiconductor consists of a free electron gas (with an effective mass m^*), which has an energy gap above the Fermi surface. All other effects of the crystal structure are ignored.

Penn has shown that the Callaway model of a semiconductor gives an infinite value for the static dielectric constant because this model does not allow for the formation of standing waves at the Brillouin-zone boundaries. He has also shown that the neglect of umklapp processes leads to serious error. For this reason, Penn has chosen a third model, the nearly-free-electron model isotropically extended to three dimensions, which allows for the formation of standing waves at the zone edge, and for the possibility of umklapp processes.

Using Penn's wave-number-dependent dielectric function for Si, Azuma and Shindo⁸ have calculated the spatial dependence of this quantity. An identical calculation has been performed by Okuro and Azuma⁹ for Ge.

A more refined calculation of the wave-number-dependent dielectric function of Si and Ge has been performed by Nara,^{22,23} who took into account the detailed form of the energy band structure of these semiconductors. Nara has calculated the wave-vector-dependent dielectric function numerically along the three principal directions [100], [110], and [111]. His results show that, apart from smaller values of the magnitude of the wave vector, the dielectric function is roughly the same in all three directions.

Nara has also found that the effect of core states on the static dielectric constant is negligibly small, and that the same is true concerning the effect of the higher bands. Finally, it is mentioned, that another contribution to the dielectric function, namely, that resulting from bound exciton states is neglected in Nara's calculations both for Si, and for Ge, on the assumption that it is very small.

In summary, it can be said that despite the anisotropy of the dielectric function at small values of the magnitude of the wave vector, Nara's calculations confirm the principle features of Penn's model.

Srinivasan,²⁴ has reconsidered Penn's model in

detail, and extended his calculations for the model dielectric function for larger values of the magnitude of the wave vector. (He has also corrected some algebraic errors in Penn's formulas.) Srinivasan has evaluated the dielectric function both from the normal, and from the umklapp processes. His findings are interesting, inasmuch as they show that the contribution from umklapp processes is most important at small values of the magnitude of the wave vector which is precisely the region where Nara's more realistic calculations show the most pronounced anisotropy in the [100], [110], and [111] directions. Srinivasan, however, cautions that in order to be certain that Nara's results are more accurate than his, it would be necessary to repeat Nara's calculations with more attention paid to details at large values of the magnitude of the wave vector. This, however, does not seem to have been done yet.

Recently Chadi and White²⁵ used a different approach, based on the tight-binding model, to evaluate the dielectric function for Si. Their result for this quantity seems to give a somewhat lower value at all values of the magnitude of the wave vector than that of Srinivasan, but the general dependence of the dielectric function on the wave vector appears to be the same.

Calculations of the dielectric function for Si, Ge, GaAs, and ZnSe have also been performed by Walter and Cohen²⁶ on the basis of a pseudopotential method using the same model as Nara. They find a fair agreement with Srinivasan's calculations but do not find the anisotropy which characterizes Nara's results. Walter and Cohen find that the dielectric function in the [100] direction is slightly less than that in the other directions.

In addition, the results of Walter and Cohen show the dielectric function to be a monotonically decreasing function of the magnitude of the wave vector, a feature which is not present in the results of Srinivasan or Nara. The slight maxima in the dielectric function, occurring at small values of the magnitude of the wave vector in these calculations, are assumed to arise from approximations in the computations.

An examination of the Penn model by Heine and Jones²⁷ supports the isotropic feature.

Brust²⁸ has generalized the Penn model to include more than one gap. His two-gap calculations for Si and Ge, just like those of Walter and Cohen, show the dielectric function to be a monotonically decreasing function of the magnitude of the wave vector. Otherwise, his results at larger values of the wave vector agree fairly well with those of Walter and Cohen and Nara.

Finally, it is mentioned that for Si Walter and Cohen²⁹ have calculated the frequency- and wave-vector-dependent dielectric function using a pseudo-

potential method. A similar calculation for Ge, GaAs, and ZnSe has been carried out by Sramek and Cohen.³⁰ These last authors have also recalculated the wave-vector-dependent dielectric function for Ge, on the basis of the Penn model, but without the analytical simplifications of Penn. It was found that the dielectric function they obtained agrees fairly well with the results of Walter and Cohen.

To round out the discussion on the spatial dielectric function, it is mentioned that Penn's model has also been applied to solids other than semiconductors. The dielectric screening of the electron-hole interaction in solid rare gases has been considered by Hermanson³¹ in connection with the theory of exciton and impurity states in these materials. Hermanson's spatial dielectric function for the rare-gas crystals, considered as isotropic insulators, is, however, somewhat simpler than the analytical expression used in this paper for Si and Ge inasmuch as it contains only one exponential term for $1/\kappa(r)$.

V. CONCLUDING COMMENTS

All these calculations of the dielectric function have one feature in common:

A fair agreement with each other. On this basis, it seems reasonable to conclude that our use of the spatial dielectric function, resulting from the Penn model, is probably sufficiently good. Much more reliable calculations on the anisotropy of the dielectric function are needed, in the author's opinion, to warrant the derivation of a sort of an average impurity-ion potential^{32,33} which could then be used in theories of ionized-impurity scattering.

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APPENDIX: DERIVATION OF POISSON'S EQUATION FOR A MEDIUM WITH SPATIALLY-VARIABLE DIELECTRIC CONSTANT

The replacement of the static dielectric constant κ_0 by the dielectric function $\kappa(r)$ in Eq. (8) needs justification. It will now be shown that Eq. (18) can be viewed as the asymptotic form of Poisson's equation for a medium characterized by a spatially-variable dielectric constant.

We start from the definition of the electric displacement \vec{D} , namely, from

$$\vec{D} = \kappa_0 \vec{E}, \quad (\text{A1})$$

where \vec{E} is the electric field, and replace κ_0 by $\kappa(r)$, giving

$$\vec{D}(r) = \kappa(r) \vec{E}(r). \quad (\text{A2})$$

One of Maxwell's equations states that

$$\vec{\nabla} \cdot \vec{D} = 4\pi\rho, \quad (\text{A3})$$

where ρ is the screening charge density, if \vec{E} is the electric field of a donor ion in the medium.

Using the identity

$$\vec{\nabla} \cdot [\kappa(r)\vec{E}(r)] = [\vec{\nabla}\kappa(r)] \cdot \vec{E}(r) + \kappa(r)[\vec{\nabla} \cdot \vec{E}(r)], \quad (\text{A4})$$

we can write Eq. (A3), upon consideration of Eq. (A2), as

$$\vec{\nabla}\kappa(r) \cdot \vec{E}(r) + \kappa(r)\vec{\nabla} \cdot \vec{E}(r) = 4\pi\rho(r). \quad (\text{A5})$$

Since we know that

$$\vec{E}(r) = -\vec{\nabla}\phi(r), \quad (\text{A6})$$

where ϕ is the potential of a donor ion in the medium, we can rewrite Eq. (A5), considering that

$$\vec{\nabla} \cdot \vec{\nabla}\phi(r) = \nabla^2\phi(r), \quad (\text{A7})$$

as

$$\vec{\nabla}\kappa(r) \cdot [-\vec{\nabla}\phi(r)] - \kappa(r)\nabla^2\phi(r) = 4\pi\rho(r). \quad (\text{A8})$$

We can rearrange Eq. (A8) to read

$$\nabla^2\phi(r) = -\frac{4\pi\rho(r)}{\kappa(r)} + \frac{\vec{\nabla}\kappa(r) \cdot [-\vec{\nabla}\phi(r)]}{\kappa(r)}. \quad (\text{A9})$$

Equation (A9) is Poisson's equation in a medium with a spatially-variable dielectric constant. It differs from Eq. (18) by the presence of the term

$$T(r) = \frac{\vec{\nabla}\kappa(r) \cdot [-\vec{\nabla}\phi(r)]}{\kappa(r)}. \quad (\text{A10})$$

We shall now proceed with the investigation of the term T , defined in Eq. (A10). In spherical polar coordinates r, θ, φ , we have for the numerator of T

$$\begin{aligned} \vec{\nabla}\kappa(r) \cdot [-\vec{\nabla}\phi(r)] = & -\left(\frac{\partial\kappa}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial\kappa}{\partial\theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial\kappa}{\partial\varphi}\hat{\varphi}\right) \\ & \cdot \left(\frac{\partial\phi}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial\phi}{\partial\theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial\phi}{\partial\varphi}\hat{\varphi}\right), \end{aligned} \quad (\text{A11})$$

where $\hat{r}, \hat{\theta}, \hat{\varphi}$ are unit vectors. Considering that $\kappa(r)$ does not depend on θ and φ , and that neither does the potential ϕ , we find from Eq. (A11) that

$$\vec{\nabla}\kappa(r) \cdot [-\vec{\nabla}\phi(r)] = -\frac{d\kappa(r)}{dr} \frac{d\phi(r)}{dr}. \quad (\text{A12})$$

Using Eq. (A12), we can express Eq. (A9) as

$$\phi'' + \frac{2}{r}\phi' = -\frac{4\pi\rho(r)}{\kappa(r)} - \frac{1}{\kappa(r)} \frac{d\kappa(r)}{dr} \phi'. \quad (\text{A13})$$

We now focus attention on the term

$$T = -\frac{1}{\kappa(r)} \frac{d\kappa(r)}{dr} \phi'. \quad (\text{A14})$$

Using for $\kappa(r)$ the expression given in Eq. (15), the differentiation is performed and we obtain

$$T = -\frac{\alpha e^{-\alpha r} - A\beta e^{-\beta r} - B\gamma e^{-\gamma r}}{e^{-\alpha r} + A(1 - e^{-\beta r}) + B(1 - e^{-\gamma r})} \phi', \quad (\text{A15})$$

or

$$T = -h_2(r)\phi', \quad (\text{A16})$$

where we have denoted the coefficient of ϕ' in Eq. (A15) by $h_2(r)$. We find that at $r=0$, and at $r=\infty$ it assumes the values

$$[h_2(r)]_{r=0} = \alpha - A\beta - B\gamma \quad (\text{A17})$$

and

$$[h_2(r)]_{r=\infty} = 0. \quad (\text{A18})$$

With the aid of Eqs. (A17) and (A18), we see from Eq. (A15), that $h_2(r)$ rapidly drops from a constant value at $r=0$ to a value of 0 as r increases. We recall that the expansion of the Fermi-Dirac integral in Eq. (3) is meaningful only when ϕ is small, which happens at large values of r . For this reason, we may justifiably drop the term T in Eq. (A13) and view the resulting equation, which has been used in this paper, as the asymptotic form of Poisson's equation for the potential of a donor ion in a medium with a spatially-variable dielectric constant. This then is the justification of simply replacing the static dielectric constant in Eq. (8) by the spatial dielectric function. It is then also the justification for our assumption that the not pointlike screening charge density is itself screened the same way as a point charge is screened by the dielectric function. This conclusion appears plausible, since a spatially extended but spherically symmetric charge distribution, when viewed from a large distance, should resemble a point charge.

It is fortunate that the term T can be, asymp-

totically, neglected. Otherwise, the solution of the differential equation in Eq. (A13) would appear to present intractable difficulties.

Another argument for dropping the term T in Eq. (A13) can also be advanced, based on the relative importance of the coefficients of ϕ' in Eq. (A13). Denoting the coefficient of ϕ' on the left-hand side of Eq. (A13) by $h_1(r)$, i. e., introducing

$$h_1(r) = 2/r, \quad (\text{A19})$$

we find that the quantity

$$\frac{h_2}{h_1} = \frac{r(\alpha e^{-\alpha r} - A\beta e^{-\beta r} - B\gamma e^{-\gamma r})}{2[e^{-\alpha r} + A(1 - e^{-\beta r}) + B(1 - e^{-\gamma r})]} \quad (\text{A20})$$

at $r=0$, and at $r=\infty$ assumes the values

$$(h_2/h_1)_{r=0} = 0 \quad (\text{A21})$$

and

$$(h_2/h_1)_{r=\infty} = 0. \quad (\text{A22})$$

Equations (A21) and (A22) tell us that the term T is unimportant both at very small, and at very large values of r . The structure of Eq. (A20), however, suggests that the magnitude of h_2/h_1 , goes through a maximum at some finite value of r . Owing to the predominance of the exponentials over r , however, this maximum should hover close to zero, permitting us to infer that the term $h_2\phi'$, relative to the term $h_1\phi'$, is not important.

As a final comment, we might add that, perhaps, it is possible to approximate $h_2(r)$ by a simple analytical function and then search for a variational principle that could lead to an approximate solution of the complete modified Poisson's equation. This step requires formidable effort and, in the author's opinion, would only be justified should one be able to agree on the most reliable analytical approximation to the physically best spatial dielectric function.

*Part of this work has been done when the author was a visiting lecturer at the UCLA.

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