

## Nonlinear dielectric response to a point-donor impurity of an electron-gas-model semiconductor that includes the effect of the Dirac-Slater exchange correlation

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The Thomas-Fermi statistical theory, including the Dirac-Slater local-density treatment of exchange correlation, has been applied to the problem of nonlinear screening of a donor point charge embedded in an electron-gas-model semiconductor. The nonlinear screening equation is solved numerically, giving spatial dielectric functions and screening radii with exchange-correlation strength and ion-charge state as parameters. Illustrations and tabulations of these results are given for five semiconductors, four ion charges, and two nonzero values of the exchange-correlation strength corresponding to the Kohn-Sham and Slater exchange potentials. A variational principle equivalent of the nonlinear equation leads to approximate analytical expressions for the spatial dielectric functions which are in close agreement with the exact results. Variational parameters are given for a subset of the semiconductors and charge states. Dielectric functions of silicon are used to illustrate typical comparisons between the two methods of solution.

### I. INTRODUCTION

This paper is concerned with nonlinear screening of an ionized point donor embedded in an electron-gas model semiconductor involving exchange and correlation in the Dirac-Slater  $X\alpha$  approximation. Two familiar procedures for developing the associated nonlinear equation for dielectric screening of the impurity have been outlined in a previous paper.<sup>1</sup> One of these is based on the original Thomas-Fermi statistical theory but modified to include exchange and correlation. This approach, due to Mott,<sup>2</sup> starts from the uniform-electron-gas relation between the electron density  $n$  and the Fermi momentum  $k_F$  and applies it locally at  $r$  to the inhomogeneous system that results when the point charge is introduced into the semiconductor. A local Fermi energy  $E_F(r)$  is expressed in terms of  $k_F(r)$  in the same way that the uniform-gas Fermi energy  $E_F$  is written in terms of  $k_F$ . In the present instance,  $E_F$  contains kinetic- and potential-energy terms proportional to  $k_F^2$  and  $k_F$ , respectively. It then remains to set up the classical equation for the fastest electron moving in the common screened potential  $V(r)$  with local kinetic and exchange-correlation energy  $E_F(r)$ . This equation is a statement of the constancy of the Fermi energy  $E_F$  (chemical potential at absolute zero) throughout the system, and includes the boundary condition,  $n(R)=n$ , on the screening charge density, where  $R$  is the finite radius of incomplete screening. The basic nonlinear relation between  $n(r)$  and  $V(r)$  is given by this classical equation. Self-consistency requires that  $V(r)$  satisfy Poisson's equation with a charge distribution given in terms of the displacement of  $n(r)$  from the unperturbed electron density. This nonlinear differential equation is the fundamental Thomas-Fermi-Dirac screening equation in the  $X\alpha$  approximation. In the following, TF, TFD, and TFDS shall denote Thomas-Fermi (no exchange and correlation), Thomas-

Fermi-Dirac (pure exchange), and Thomas-Fermi Dirac-Slater (exchange and correlation in the  $X\alpha$  approximation), respectively.

The nonlinear TFDS screening equation may also be obtained from an equivalent variational principle of the modified TF theory, as outlined by March.<sup>3</sup> Minimization of the total ground-state energy of the system of valence electrons (plus any external potentials) with respect to  $n(r)$ , and with a constraint on the total number of electrons, leads to an Euler equation which expresses the constancy of the chemical potential and the boundary condition on the screening charge. The latter is incorporated in the theory by using a Lagrange multiplier (related to the fixed number of electrons) of the form  $E_F + V(R)$ . The Euler equation embodies the nonlinear relation between  $n(r)$  and  $V(r)$  as before.

The spatial dielectric function  $\bar{\epsilon}(r)$  is defined as the ratio of the bare Coulomb potential,  $-Z/r$ , to the screened potential,  $V(r)$ , set up around the impurity point charge. Its properties include  $\bar{\epsilon}(0)=1$  and  $\bar{\epsilon}(r)=\epsilon(0)$ , where  $\epsilon(0)$  is the macroscopic dielectric constant for  $r \geq R$ . Linearization of the TFDS screening equation yields the simple analytical form of  $\bar{\epsilon}(r)$  previously derived in the linearized TF context.<sup>4</sup> In this approximation, exchange-correlation effects enter the potential  $V(r)$  through a parameter, called  $q$  [see Eq. (12)], which reduces to the usual TF screening length when exchange and correlation are absent. Reference 1 employed the linearized screening function in a variational calculation of donor ionization energy with ion charge state  $Z$  and exchange-correlation strength  $\alpha$  as parameters. It is of interest to extend this application and others to the nonlinear regime. The present paper<sup>5</sup> makes a first step in that direction by developing numerical and approximate analytical solutions of the nonlinear screening equation in the  $X\alpha$  scheme. The former is taken up in Sec. II for the potentials of donor point charges in diamond, silicon, germani-

um, gallium arsenide, and gallium phosphide. Four positive charges  $Z=+1,+2,+3,+4$  and three values of  $\alpha$ , namely,  $\alpha=0.0$  (no exchange interaction),  $\alpha=0.67$  (Kohn-Sham exchange potential), and  $\alpha=1.0$  (Slater exchange potential) are used in illustrating numerical results for screening radii and spatial dielectric functions. The effect of exchange and correlation on these quantities is seen *vis-à-vis* predictions of the TF screening theory.

A variational principle equivalent of the nonlinear TFDS screening equation is devised in Sec. III. This approach gives approximate analytical expressions for  $\bar{\epsilon}(r)$  containing three variational parameters. Spatial dielectric functions of silicon for two positive charges ( $Z=+1,+3$ ) and three values of  $\alpha$  are shown in graphical form to be in very close agreement with the numerical results. Except for the time-consuming work involved in the numerical search for extrema, the ease with which the  $\bar{\epsilon}(r)$  are secured in the variational method surpasses the exact approach, which calls for a tedious numerical matching of the potential and the electric field at  $r=R$ . This paper employs the atomic system of units in which the unit of length is the first bohr orbit ( $a_0$ ) and the unit of energy is the hartree (twice the rydberg). The electronic charge ( $e$ ), mass ( $m$ ), and action ( $\hbar$ ) are set equal to unity.

## II. NUMERICAL SOLUTIONS OF THE NONLINEAR SCREENING EQUATION FOR POSITIVE CHARGES

Numerical solutions of the nonlinear TFD screening equation for positive charges have been obtained in an earlier paper.<sup>6</sup> Corresponding spatial dielectric functions and screening radii for diamond, silicon, and germanium

are recorded there in graphical and tabular forms, respectively. Reference 6 also includes a graphical comparison of the TF and TFD spatial dielectric functions for the same semiconductors in the nonlinear regime. That application led to the conclusion that exchange causes a further contraction of the TF screening radius of a positive point-charge impurity. This effect is already evident in the linearized TF and TFD screening theories where the spatial dielectric functions are obtained in simple analytical form. The nonlinear TFDS scheme provides a framework for investigating the behavior of  $R$  and  $\bar{\epsilon}(r)$  as continuous functions of the exchange-correlation strength for various positive charges  $Z$ . This program is carried out in this section for the five semiconductors mentioned above. In the present work, site dependency<sup>7</sup> of the dielectric functions of the compound semiconductors is not considered. It may be taken into account by employing effective donor charges due to the partial ionicity of the chemical bonds on one site (Ga) or the other (As or P).

There are two distinct regions of interest in the space around a donor impurity. One of these contains the dispersive dielectric response of the semiconductor, and extends from the point probe located at the origin ( $r=0$ ) to the screening distance  $R$ . The second region is the rest of space from  $R$  to infinity, at each point of which the bare Coulomb potential is screened by the static macroscopic dielectric constant. Thus

$$V(r) = -\frac{Z}{\epsilon(0)r}, \quad r \geq R. \quad (1)$$

In the screening region, the impurity potential satisfies the nonlinear differential equation

$$\nabla^2 V(r) = \frac{2^{7/2}}{3\pi} \left\{ \left[ \frac{3\alpha}{2^{3/2}\pi} + \left( \frac{9\alpha^2}{8\pi^2} + E_F \right)^{1/2} \right]^3 - \left[ \frac{3\alpha}{2^{3/2}\pi} + \left( \frac{9\alpha^2}{8\pi^2} + E_F + V(R) - V(r) \right)^{1/2} \right]^3 \right\}, \quad r \leq R. \quad (2)$$

The desired solution of Eq. (2) approaches  $-Z/r\epsilon(0)$  and  $-Z/r$  as  $r$  approaches  $R$  and the origin, respectively. Continuity of the potential and the electric field at  $r=R$  completes the definition of the donor problem. Equation (2) is the TFDS generalization of previous nonlinear equations for the screened impurity potential, including the TF and TFD theories as special cases. Input parameters, for a given semiconductor, are the Fermi momentum  $k_F$ , the dielectric constant  $\epsilon(0)$ , the point-ion charge  $Z$ , and the exchange-correlation strength  $\alpha$ . The Fermi energy  $E_F$  is expressed in terms of  $k_F$  and  $\alpha$  by the uniform-electron-gas relation

$$E_F = \frac{k_F^2}{2} - \frac{3\alpha}{2\pi} k_F. \quad (3)$$

With given input parameters and a starting value for  $R$ , Eq. (2) is solved numerically inward, matching the potential and its derivative at  $r=R$ . The screening radius is varied until the solution has the correct behavior at the origin. This procedure was implemented with a Runge-

Kutta-Vernier fifth- and sixth-order routine. Matching of dependent variables to satisfy required behavior at the origin or continuity at  $r=R$  was rigorously enforced to within  $10^{-4}$ . Screening radii found for each semiconductor are listed in Table I. Monovalent, divalent, trivalent, and tetravalent donor ions, and three values of the exchange-correlation parameter corresponding to no exchange and correlation ( $\alpha=0.0$ ), the Kohn-Sham potential ( $\alpha=0.67$ ), and the Slater potential ( $\alpha=1.0$ ) are considered. Results for GaAs and GaP are in excellent agreement with recent<sup>8</sup> numerical calculations which also neglect partial ionicity of the chemical bonds on a site. It is clear from Eqs. (2) and (3) that in order to solve the TF and TFD problems it is only necessary to set  $\alpha=0.0$  and  $0.67$ , respectively, in the input data file of the computer program for the TFDS case. For some inscrutable reason, the authors of Ref. 8 fail to see that  $E_F$ , in the TFD case of Ref. 6, may be expressed as  $E_F = (k_F^2/2) - \gamma k_F \sqrt{2}$  where the exchange parameter  $\gamma$  is an abbreviation for  $(1/\pi\sqrt{2})$ , and that merely setting  $\gamma=0$  in the computer program for the TFD case recovers

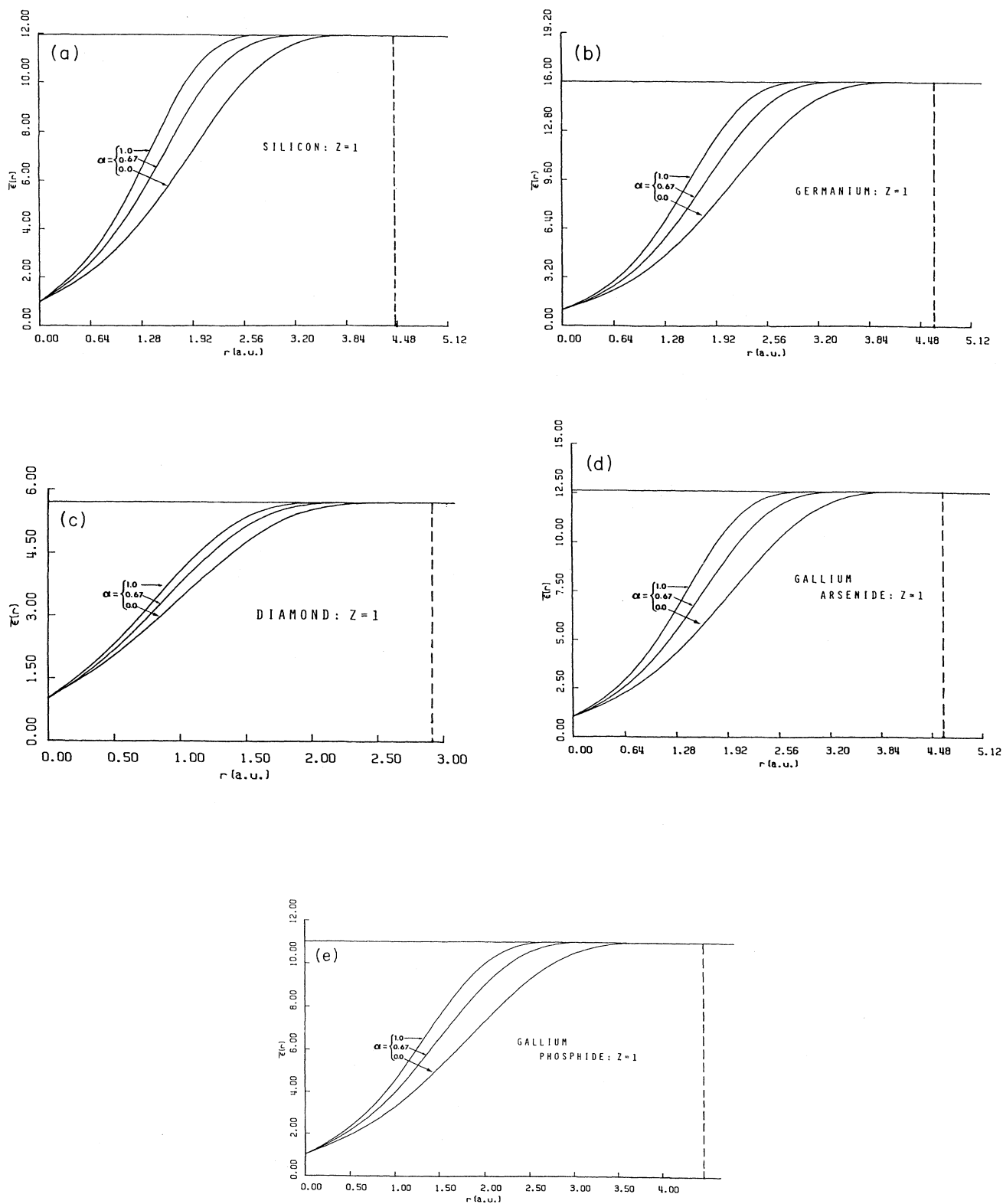


FIG. 1. Exact spatial dielectric functions for (a) silicon, (b) germanium, (c) diamond, (d) gallium arsenide, and (e) gallium phosphide with exchange-correlation strength as parameter, for the monovalent ion-charge state in the nonlinear regime of TFDS screening.

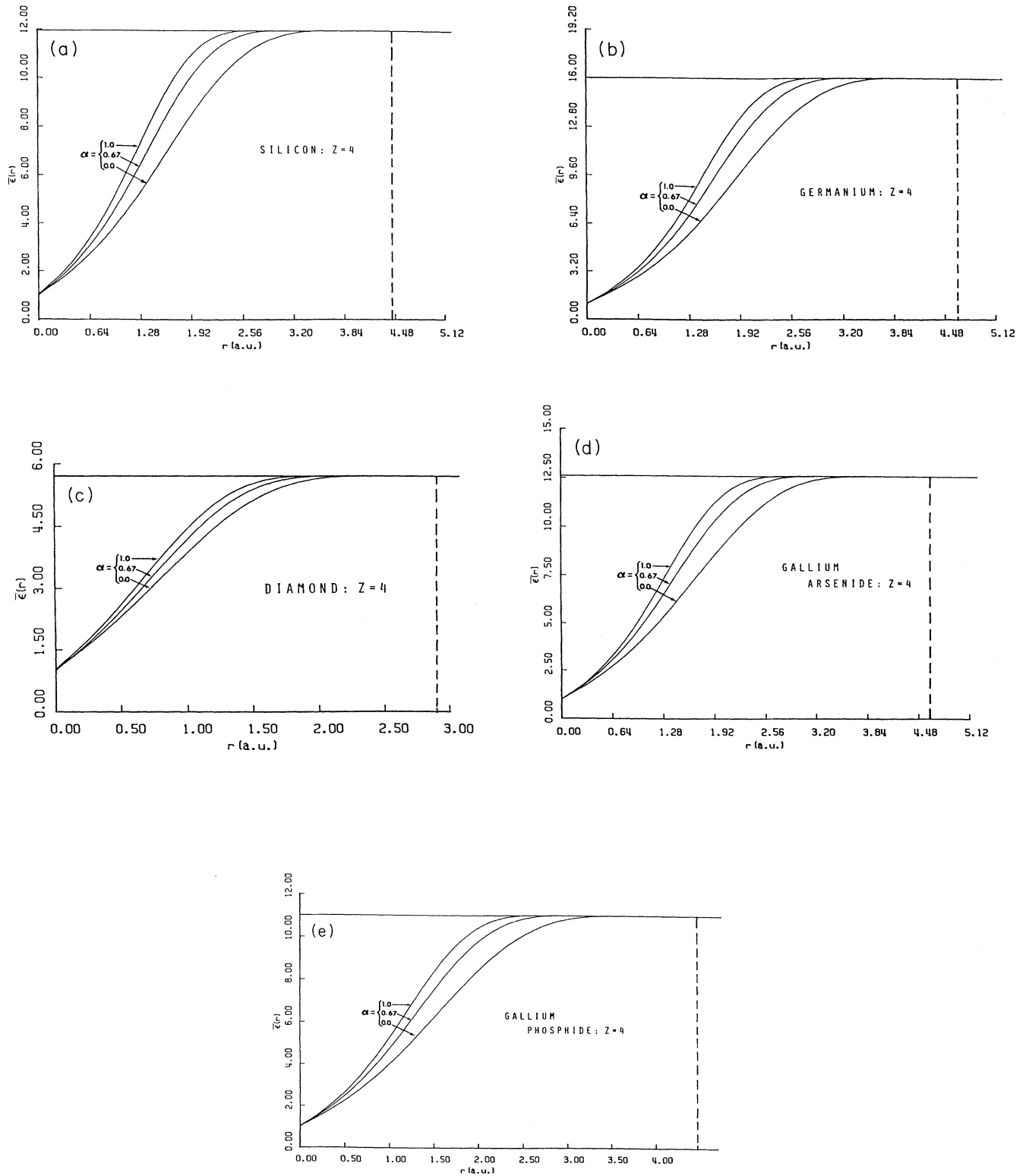


FIG. 2. Exact spatial dielectric functions for (a) silicon, (b) germanium, (c) diamond, (d) gallium arsenide, and (e) gallium phosphide with exchange-correlation strength as parameter, for the tetraivalent ion-charge state in the nonlinear regime of TFDS screening.

TABLE I. Screening radii  $R$  for Si, Ge, diamond, GaAs, and GaP in the nonlinear regime of TFDS screening for four ion-charge states,  $Z$ , and three values of the exchange-correlation strength,  $\alpha$ .

| Semiconductor | $\alpha$ | $Z$  |      |      |      |
|---------------|----------|------|------|------|------|
|               |          | +1   | +2   | +3   | +4   |
| Si            | 0.0      | 4.06 | 3.92 | 3.80 | 3.74 |
|               | 0.67     | 3.34 | 3.24 | 3.17 | 3.11 |
|               | 1.0      | 3.04 | 2.90 | 2.80 | 2.76 |
| Ge            | 0.0      | 4.33 | 4.21 | 4.12 | 4.02 |
|               | 0.67     | 3.60 | 3.50 | 3.43 | 3.37 |
|               | 1.0      | 3.16 | 3.11 | 3.06 | 3.00 |
| Diamond       | 0.0      | 2.64 | 2.57 | 2.50 | 2.44 |
|               | 0.67     | 2.34 | 2.27 | 2.22 | 2.18 |
|               | 1.0      | 2.16 | 2.11 | 2.04 | 2.02 |
| GaAs          | 0.0      | 4.19 | 4.05 | 3.95 | 3.86 |
|               | 0.67     | 3.42 | 3.32 | 3.25 | 3.19 |
|               | 1.0      | 2.96 | 2.90 | 2.87 | 2.84 |
| GaP           | 0.0      | 3.98 | 3.85 | 3.74 | 3.66 |
|               | 0.67     | 3.27 | 3.18 | 3.10 | 3.04 |
|               | 1.0      | 2.87 | 2.80 | 2.75 | 2.71 |

the TF form of  $E_F$ .

Spatial dielectric functions for all five semiconductors have been generated numerically and graphically, but for economy of presentation, only the monovalent and tetravalent results are shown in Figs. 1 and 2, respectively. The divalent and trivalent curves for each value of  $\alpha$  lie between the area bordered by the  $Z = +1$  and  $+4$  curves. It has already been established in the TFD theory<sup>6</sup> of screening that nonlinearity and exchange are more effective at reducing attractive potentials than the former acting alone. In other words, the screening electrons in the nonlinear TFD and TF theories are closer to the point-donor ion in the former case. In the present TFDS application, it is found that a continuous increase in  $\alpha$  causes a steady decrease in the screening radius, meaning that the screening electrons more closely approach the impurity. It may be considered that correlation energy between electrons of parallel spin effectively increases the numerical coefficient of  $k_F$  in the TFD expression for  $E_F$ . The Dirac-Slater method is a relatively practical way to account for correlation within the local exchange-correlation approximation. The results in Table I and Figs. 1 and 2 show the effect of exchange correlation on the dielectric response of the semiconductors. The inclusion of this feature and its numerical outcome represent a generalization of earlier calculations

performed in the TF (Ref. 9) and TFD (Refs. 6 and 8) frameworks.

### III. VARIATIONAL METHOD AND APPROXIMATE ANALYTICAL SOLUTIONS OF THE NONLINEAR SCREENING EQUATION FOR DONOR POINT CHARGES

This section is concerned with the development of approximate analytical solutions of the nonlinear TFDS equation for positive point charges embedded in various semiconductors. A variational principle of the variable-domain type is used for this purpose. The procedure involves finding a function  $F$  which provides an Euler-Lagrange equation equivalent of the nonlinear TFDS equation, and also a quantity  $G$  which accounts for the variation of the domain. It then remains to choose a convenient trial wave function and to secure the extremum of a functional  $J$  with respect to the parameters in the trial function. The functional  $J$  is the quantity  $G$  plus the integral of  $F$  over the independent variable  $r$  between the fixed lower limit,  $r=0$ , and a variable upper limit,  $r=R$ . The aim is to obtain the potential and spatial dielectric function in closed analytical form. These expressions may then be used in considering other semiconductor problems, such as ionized impurity scattering and shallow-donor ionization energy. Applications of the variational technique in this context have been concerned with the nonlinear TF equation for positive and negative point charges in elemental<sup>10</sup> and compound<sup>7</sup> semiconductors.

In the interest of finding the function  $F$ , it is useful to redefine the mathematical problem posed by the equations for  $V(r)$ , in the two regions under consideration, and their boundary and matching conditions. Equation (1) implies that  $V(r)$  satisfies Laplace's equation beyond the screening radius, while inside that radius  $V(r)$  is described by Eq. (2). Consider the function

$$\psi(r) = r [V(r) - V(R)] . \quad (4)$$

It follows from Eqs. (1) and (4) that

$$\psi(r) = -\frac{Z}{\epsilon(0)} \left[ 1 - \frac{r}{R} \right] , \quad r \geq R . \quad (5)$$

In this region, the second derivative (double prime) of  $\psi(r)$  with respect to  $r$  vanishes, as expected. It is also seen that the matching condition on the potential at  $r=R$  becomes simply  $\psi(R)=0$ . Equations (2) and (4) readily show that the nonlinear differential equation satisfied by  $\psi(r)$  inside the screening radius is given by

$$\psi''(r) - \frac{2^{7/2}r}{3\pi} \left\{ \left[ \frac{3\alpha}{2^{3/2}\pi} + \left( \frac{9\alpha^2}{8\pi^2} + E_F \right)^{1/2} \right]^3 - \left[ \frac{3\alpha}{2^{3/2}\pi} + \left( \frac{9\alpha^2}{8\pi^2} + E_F - \frac{\psi(r)}{r} \right)^{1/2} \right]^3 \right\} = 0, \quad r \leq R . \quad (6)$$

The boundary condition on  $V(r)$  as  $r$  approaches the origin demands that  $\psi(r)$  approach  $-Z$  in that limit.

The function  $F = F(\psi, \psi', r)$  may now be found by writing it as the sum of two parts, one given simply by  $-\frac{1}{2}(\psi')^2$ , and the other involving  $r$  and  $\psi$ . In the Euler-Lagrange equation for  $F$ , namely,

$$\frac{d}{dr} \left[ \frac{\partial F}{\partial \psi'} \right] - \frac{\partial F}{\partial \psi} = 0, \quad (7)$$

The first part of  $F$  will give the second derivative term in Eq. (6). The partial derivative of the second part of  $F$  with respect to  $\psi$  must equal the remaining terms in Eq. (6). Integration of this relation yields the second part of  $F$ . The final result for  $F$  may be expressed as

$$F = -\frac{1}{2}(\psi')^2 - \frac{2^{7/2}r}{3\pi} \left\{ \left[ \frac{3\alpha}{2^{3/2}\pi} + \left( \frac{9\alpha^2}{8\pi^2} + E_F \right)^{1/2} \right]^3 - \frac{9\alpha}{2^{3/2}\pi} \left[ \frac{12\alpha^2}{8\pi^2} + E_F \right] \right\} \Psi \\ - \frac{2^{7/2}r}{3\pi} \left[ \frac{3}{2r} \left[ \frac{3\alpha}{2^{3/2}\pi} \right] \psi^2 + 2r \left[ \frac{9\alpha^2}{8\pi^2} \right] \left[ \frac{9\alpha^2}{8\pi^2} + E_F - \frac{\psi}{r} \right]^{3/2} + \frac{2r}{5} \left[ \frac{9\alpha^2}{8\pi^2} + E_F - \frac{\psi}{r} \right]^{5/2} \right]. \quad (8)$$

It is easy to verify that  $F$  given by Eq. (8) satisfies Eq. (7) and, indeed, the resulting equation is Eq. (6), as expected. In view of the validity of Eq. (7), the first variation of the integral of  $F$  contained in the functional  $J$  yields two nonzero terms due to the variation of the domain. The quantity  $\delta G$  is defined as the negative of these terms, namely,

$$\delta G = \psi' \delta \psi|_{r=R} - F|_{r=R} \delta R. \quad (9)$$

Thus the variational principle can be stated as  $\delta J = 0$ . The right-hand side of Eq. (9) is evaluated with expressions for  $\psi$ ,  $\psi'$ , and  $\delta \psi$ , provided by Eq. (5), at the boundary point  $r = R$ . It then remains to recognize that the resulting form of the right-hand side of Eq. (9) may be rewritten as a variation of the desired quantity

$$G = \frac{1}{2} \left[ \frac{Z}{\epsilon(0)} \right]^2 \frac{1}{R} \\ + \frac{2}{3} \left[ \frac{2^{7/2}}{3\pi} \right] \left[ \frac{1}{5} \left[ \frac{9\alpha^2}{8\pi^2} + E_F \right]^{5/2} \right. \\ \left. + \frac{9\alpha^2}{8\pi^2} \left[ \frac{9\alpha^2}{8\pi^2} + E_F \right]^{3/2} \right] R^3. \quad (10)$$

The next step involves the choice of the trial function  $\psi$ . The adopted  $\psi$  must satisfy the boundary condition at the origin and the matching condition at  $R$  given, respectively, by  $\psi(0) = -Z$  and  $\psi(R) = 0$ . It has been shown in Ref. 6 that the linearized form of the nonlinear TFD equation is invalid for values of  $r$  less than a critical value, say,  $r_c$ . To visualize the meaning of  $r_c$ , it may be compared with  $R$  and the nearest-neighbor distance  $a$ . For example, when  $Z = +1$  in the case of silicon,  $r_c/R = 0.31$  and  $r_c/a = 0.24$ . The corresponding ratios in the linearized TF theory are  $r_c/R = 0.20$  and  $r_c/a = 0.19$ .

The above considerations suggest that the trial function may be expressed as the product of two factors, one embodying the form of the solution of the linear TFD equation, while the other modifies this form for small  $r$  in the region  $0 \leq r \leq r_c$ . With this motivation, the trial function is written as

$$\psi(r) = [(1-\lambda) + \lambda e^{-r/r_c}] \left[ \frac{-Z \sinh[q(R-r)]}{\sinh(qR)} \right], \quad (11)$$

where  $\lambda$  and  $r_c$  are variational parameters, and  $q$  is given by

$$q = \left[ \frac{4k_F}{\pi} \left[ \frac{k_F}{k_F - \frac{3\alpha}{2\pi}} \right] \right]^{1/2}. \quad (12)$$

Note that the boundary condition at the origin and the matching condition at  $R$  are satisfied by Eq. (11). For  $\lambda = 0$ , this trial function formally reduces to the solution of the linear TFD equation. When Eqs. (5) and (11) are used in the matching condition of  $\psi'$  at  $r = R$ , the three quantities  $\lambda$ ,  $r_c$ , and  $R$  are joined in the relationship

$$\lambda = \left[ 1 - \frac{\sinh(qR)}{\epsilon(0)qR} \right] (1 - e^{-R/r_c})^{-1}. \quad (13)$$

In view of this result,  $R$  and  $r_c$  may now be taken as the variational parameters with respect to which  $J$  is an extremum.

As mentioned before,  $J$  is the sum of  $G$  and the integral of  $F$  over the region  $0 \leq r \leq R$ . In order to avoid the singularity in  $F$  at the origin, it is convenient to introduce the new variable  $\mu = \sqrt{r}$ . In that case  $J$  takes on the form

$$\begin{aligned}
J(R, r_c) = & - \int_0^{\sqrt{R}} (\psi')^2 du - 2 \left[ \frac{2^{7/2}}{3\pi} \right] \left\{ \left[ \frac{3\alpha}{2^{3/2}\pi} + \left( \frac{9\alpha^2}{8\pi^2} + E_F \right)^{1/2} \right]^3 - \frac{9\alpha}{2^{3/2}\pi} \left[ \frac{12\alpha^2}{8\pi^2} + E_F \right] \right\} \int_0^{\sqrt{R}} u^3 \psi du \\
& + 3 \left[ \frac{2^{7/2}}{3\pi} \right] \left[ \frac{3\alpha}{2^{3/2}\pi} \right] \int_0^{\sqrt{R}} u \psi^2 du - 4 \left[ \frac{2^{7/2}}{3\pi} \right] \left[ \frac{9\alpha^2}{8\pi^2} \right] \int_0^{\sqrt{R}} u^2 \left[ \left[ \frac{9\alpha^2}{8\pi^2} + E_F \right] u^2 - \psi \right]^{3/2} du \\
& - \frac{4}{5} \left[ \frac{2^{7/2}}{3\pi} \right] \int_0^{\sqrt{R}} \left[ \left[ \frac{9\alpha^2}{8\pi^2} + E_F \right] u^2 - \psi \right]^{5/2} du + \frac{1}{2} \left[ \frac{Z}{\epsilon(0)} \right]^2 \frac{1}{R} \\
& + \frac{2}{3} \left[ \frac{2^{7/2}}{3\pi} \right] \left[ \frac{1}{5} \left[ \frac{9\alpha^2}{8\pi^2} + E_F \right]^{5/2} + \frac{9\alpha^2}{8\pi^2} \left[ \frac{9\alpha^2}{8\pi^2} + E_F \right]^{3/2} \right] R^3. \tag{14}
\end{aligned}$$

This completes the formulation of a variational principle equivalent for obtaining approximate analytical solutions of the nonlinear TFDS equation for positive point charges. Given the exchange-correlation value  $\alpha$ , the point impurity charge  $Z$ , and the semiconductor, characterized by  $\epsilon(0)$  and  $k_F$ , values of the variational parameters  $R$  and  $r_c$  are sought for which  $J(R, r_c)$  is an extremum. Subsequently, these values of  $R$  and  $r_c$  are fed into the expression for the spatial dielectric function

$$\begin{aligned}
\bar{\epsilon}(r) = & \left[ [(1-\lambda) + \lambda^{-r/r_c}] \left[ \frac{\sinh[q(R-r)]}{\sinh(qr)} \right] \right. \\
& \left. + \frac{r}{\epsilon(0)R} \right]^{-1}, \tag{15}
\end{aligned}$$

which follows when its definition,  $\bar{\epsilon}(r) = -Z/rV(r)$ , is combined with Eqs. (4) and (11). In the absence of exchange correlation ( $\alpha=0$ ), the above mathematical formalism reduces *in toto* to the variational principle equivalent of the nonlinear TF screening equation.

The program of calculation described above for finding  $\bar{\epsilon}(r)$  has been implemented for some of the semiconductors involved in this investigation. All integrals appearing in Eq. (14) have been evaluated by a 20-point Gauss quadrature routine. The resulting variational parameters

TABLE II. Variational parameters  $R$ ,  $r_c$ , and  $\lambda$  for Si and Ge in the nonlinear regime of TFDS screening for two ion-charge states,  $Z$ , and three values of the exchange-correlation strength  $\alpha$ .

| $Z$       | $\alpha$ | $R$  | $r_c$ | $\lambda$ |
|-----------|----------|------|-------|-----------|
| Silicon   |          |      |       |           |
| +1        | 0.00     | 4.11 | 0.22  | 0.133     |
|           | 0.67     | 3.37 | 0.20  | 0.120     |
|           | 1.00     | 2.95 | 0.17  | 0.904     |
| +3        | 0.00     | 3.92 | 0.24  | 0.263     |
|           | 0.67     | 3.23 | 0.23  | 0.241     |
|           | 1.00     | 2.86 | 0.19  | 0.188     |
| Germanium |          |      |       |           |
| +1        | 0.00     | 4.36 | 0.20  | 0.184     |
|           | 0.67     | 3.53 | 0.17  | 0.208     |
|           | 1.00     | 3.09 | 0.14  | 0.164     |
| +2        | 0.00     | 4.22 | 0.25  | 0.254     |
|           | 0.67     | 3.47 | 0.24  | 0.258     |
|           | 1.00     | 3.04 | 0.21  | 0.244     |

$R$ ,  $r_c$ , and  $\lambda$  for silicon and germanium are listed in Table II for two point charges (for Si,  $Z=+1, +3$ ; for Ge,  $Z=+1, +2$ ) and three values ( $\alpha=0.0, 0.67, 1.0$ ) of the exchange-correlation strength. The spatial dielectric

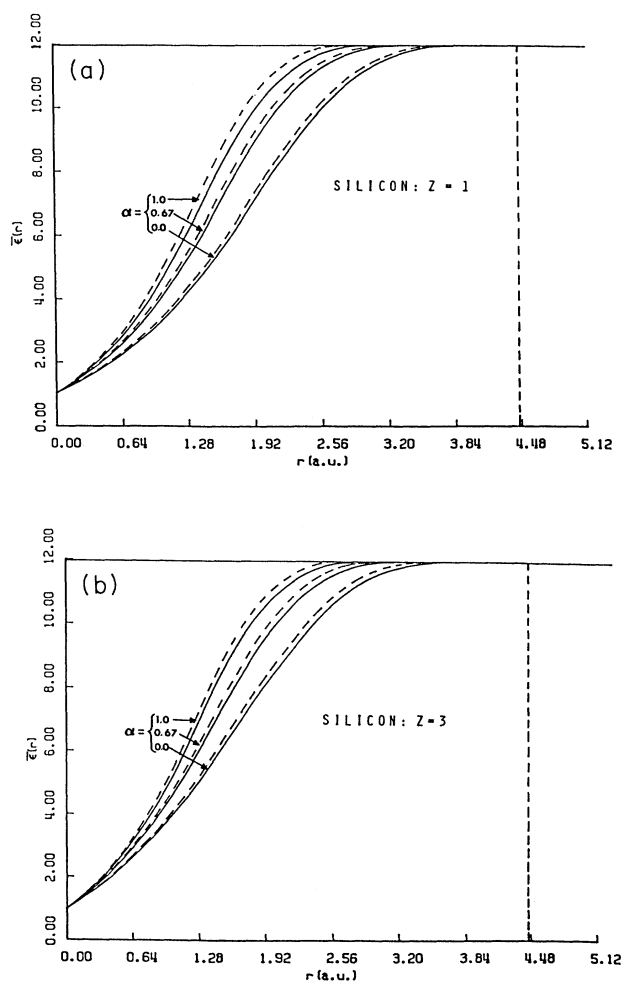


FIG. 3. Comparison of exact (solid lines) and approximate (dashed lines) spatial dielectric functions for silicon with exchange-correlation strength as parameter for (a) monovalent ( $Z=+1$ ) and (b) trivalent ( $Z=+3$ ) ion-charge states in the nonlinear regime of TFDS screening.

functions of silicon are plotted in Fig. 3, together with the numerical curves of Sec. II, shown as the dashed lines in the figures. The close agreement between the exact and approximate curves for  $\bar{\epsilon}(r)$  lends credence to the variational method of solution. Five semiconductors, four charge states, and various values of the exchange-correlation parameter corresponds to a large number of  $\bar{\epsilon}(r)$  versus  $r$  curves. Prudence dictates that specific applications be handled on an individual basis. However, the curves shown in Fig. 3 for silicon are typical of the results found in this investigation for some of the other semiconductors.

#### IV. SUMMARY

The Dirac-Slater local-density treatment of exchange correlation provides a practical way to include this effect in the TF theory of impurity screening in semiconductors and metals.<sup>4,6</sup> The ensuing nonlinear screening equation represents a generalization of the TF (Ref. 9) case of no exchange correlation and the TFD (Refs. 6 and 8) case of pure exchange. In the linear regime,<sup>1</sup> the TFDS model

yields closed analytical expressions for the potentials set up around the point probe in these materials. Boundary conditions related to incomplete (semiconductor) and complete (metal) screening lead, respectively, to Resta- and Mott-type potentials. Exchange correlation enters the linearized theory through the parameter that appears as the screening length in the case of a metal. A Resta-type potential has been used in a previous paper<sup>1</sup> to investigate the effect of exchange correlation on shallow-donor impurity ionization. With the numerical and approximate analytical solutions of the full TFDS screening equation at hand, it is now possible to study corrections to the linear theory due to nonlinearity and exchange correlation. In particular, calculation of shallow-donor ionization energy and ionized impurity scattering are applications of basic interest in this context.

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