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Thomas-Fermi-Dirac statistical theory of dispersive dielectric screening in undoped semiconductors at zero temperature

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Static dielectric screening in undoped semiconductors at zero temperature is formulated within the framework of the Thomas-Fermi-Dirac (TFD) model of a homogeneous and isotropic solid. At each point in the solid the valence electrons are treated as a degenerate gas in statistical equilibrium in the space-varying self-consistent potential of a point-charge impurity. The theory involves the electrostatic, kinetic, and exchange energies of the electrons in the development of a nonlinear TFD equation for the screened potential. The Thomas-Fermi (TF) theory of dielectric screening is recovered when exchange effects are neglected. Closed analytical expressions for the wave-vector-dependent dielectric function and the spatial dielectric function are obtained by linearization of the TFD equation and the range of validity of approximation investigated. Numerical solutions of the nonlinear TFD equation for point-charge screening show an increasing departure from linear behavior with impurity charge. These properties of the nonlinear TFD theory are already manifest in the TF scheme. A comparison between TFD- and TF-model dielectric functions shows important differences due to exchange. In the linear screening regime, it is found that impurity potentials are more effectively reduced when exchange effects are included. As a result, the TF theory compares more favorably with accurate band-structure calculations of the dielectric functions for silicon and germanium. It is expected that improvement in the TFD dielectric functions depends on extending the treatment to include correlation and/or the quantum correction. In the nonlinear regime, attractive potentials are more effectively screened in the TFD theory, while the opposite is not generally true for repulsive potentials. Finally, it is seen that donor-acceptor asymmetry is stronger in the presence of exchange effects.

I. INTRODUCTION

Simplified descriptions of the response of a semiconductor to an external static disturbance are useful for practical calculations of the physical properties of the crystal. This paper concerns the development of model dielectric functions for undoped semiconductors at zero temperature in the framework of the Thomas-Fermi-Dirac (TFD) statistical theory of linear and nonlinear impurity screening. The Thomas-Fermi (TF) -model dielectric functions obtained by Resta[1] are found to be in excellent agreement with the accurate pseudopotential random-phase-approximation calculations of Walter and Cohen[2] made in wave-vector space. An appealing aspect of the statistical approach is that dielectric functions are derived directly in configuration space, thus circumventing cumbersome Fourier transformations. The TF theory has been studied in the nonlinear regime by Cornolti and Resta,[3] and extended to deal with polar semiconductors[4] and the intervalley mixing effect on donor impurity levels and excitons in many-valley semiconductors.[5] In order to obtain analytical spatial dielectric functions, Csavinszky and Brownstein[6] have devised a variational principle equivalent of the nonlinear TF screening equation. Chao[7] defines a local screening length and derives a simple algebraic equation which yields the TF spatial dielectric function in the nonlinear regime.

The first model of a wave-vector-dependent dielectric function $\epsilon(\vec{k})$ for a semiconductor appears to be that formulated by Callaway,[8] who modified the free-electron-gas expression by inserting an energy gap between the valence and conduction bands. Penn[9] proposed a more sophisticated model by extending the nearly-free-electron gas isotropically in three dimensions, while Tosatti and Pastori-Parravicini[10] surmounted the long-wavelength difficulty in Callaway's model by requiring the f-sum rule to be obeyed. Srinivasan[11] improved on Penn's interpolation formula and obtained consistent results over the entire range of $\vec{k}$. Compared with the detailed pseudopotential calculations of Nara[12] and the accurate self-consistent-field calculations of Walter and Cohen, Srinivasan's Penn-model results give a reasonably good description of the static screening properties of semiconductors. Expressions for the wave-vector-dependent dielectric functions based on the Penn model involve complicated integrations in $\vec{k}$ space and simple k-function fits to the numerical results. A peak in $\epsilon(\vec{k})$ for small k seen by early Penn-model works[9,11,12] is thought to be a numerical artifact. Some authors[13] have been tempted to attribute the peak to a double counting of the normal processes. Detailed band-structure calculations[2] of $\epsilon(\vec{k})$ do not show this behavior. Moreover, a simple tight-binding approach[14] and a generalization[15] of the Penn model containing two energy gaps have been used to derive wave-vector-dependent dielectric functions without the hump at small k. Inkson[16] has given an especially simple expression of $\epsilon(\vec{k})$ in very close agreement with the numerical results of Ref. 2. Exact calculations[17] with the Penn model have removed all inconsistencies in the early efforts, including the failure of the frequency and wave-vector-dependent dielectric function $\epsilon(\vec{k},\omega)$ to satisfy the Kramers-Kronig relation or the f-sum rule. A more recent form of $\epsilon(\vec{k},\omega)$ proposed by Levine and Louie[18] has several desirable features, including homogeneity, isotropy, causality, particle-number conservation, and an analytic representation.

Section II introduces the degenerate-electron-gas model semiconductor and formulates the nonlinear TFD screening equation and its linearization. The linear TFD equation is solved in Sec. III and analytical expressions are obtained for the spatial and wave-vector-dependent dielectric functions. This development proceeds identically to that of Resta. Section IV presents numerical results for diamond, Si, and Ge in the linear approximation and investigates its range of validity. Comparisons are made with TF linear-response functions. TFD nonlinear-response theory for positive and negative point-charge impurities is discussed in Sec. V. Finally, in Sec. VI, numerical results illustrating nonlinear screening effects in the TFD theory are displayed for monovalent and tetravalent ions in diamond, Si, and Ge. Comparisons are made with corresponding TF predictions. Atomic units are used throughout the paper, so that e, $\hbar$, and m equal 1.

II. TFD EQUATION FOR THE SELF-CONSISTENT SCREENED POTENTIAL OF A POINT-CHARGE IMPURITY

In the absence of any external disturbance the homogeneous and isotropic model semiconductor is translationally and rotationally invariant with a uniform electron density n. The ground state of the system occupies a spherical region in momentum space of radius k_F (the valence Fermi momentum) given by

$$k_F=(3\pi^2 n)^{1/3} . \tag{1}$$

The response of the valence-electron medium to the presence of a static impurity point charge Z at the origin $(r=0)$ may be characterized by a spatial dielectric function $\bar{\epsilon}(r)$ conventionally defined as the ratio of the unscreened potential[19] $v=-Z/r$ to the self-consistent screened potential $V(r)$ set up around the point probe. Thus

$$\bar{\epsilon}(r)=v(r)/V(r), \quad r\leq R \tag{2}$$

where R is the screening radius beyond which $V(r)$ has the Coulomb form screened by the static macroscopic dielectric constant $\epsilon(0)$ of the semiconductor,

$$V(r)=v(r)/\epsilon(0), \quad r\geq R . \tag{3}$$

The TF and TFD statistical theories employ a local-density description of the degenerate electron gas in the presence of the point-charge external disturbance. It is assumed that Eq. (1) is a valid connection between the local Fermi momentum $k_F(r)$ and the screening charge density $n(r)$ at point r. In other words,

$$k_F(r)=[3\pi^2 n(r)]^{1/3} . \tag{4}$$

This approach is justified for an electron gas, which is so dense that a statistically large number of particles may be found within a region of space over which the variation of the potential is very small. In that case, thermodynamic considerations attribute a local valence Fermi energy $E_F(r)$ to the region about r. The equilibrium condition for no diffusion current of electrons is expressed by the classical energy equation

$$E_F(r)+V(r)=E_F+V(R) , \tag{5}$$

where $V(R)$ is a constant, and any change in the ambient Fermi energy E_F due to the introduction of the foreign point charge is neglected. For a degenerate electron gas of maximum momentum k_F, the energy E_F consists of the kinetic energy of the electron $k_F^2/2$, the exchange energy $-k_F/\pi$, and the correlation energy $E_c(k_F)$.[20] Since this paper is concerned with corrections to the TF theory of dielectric screening due to the effects of exchange, the correlation energy is henceforth dropped and E_F is expressed as

$$E_F=\tfrac{1}{2}k_F^2-\frac{1}{\pi}k_F , \tag{6}$$

where k_F is given by Eq. (1). It may be considered that correlation energy between electrons of parallel spin effectively increases the numerical coefficient of k_F in Eq. (6) to a value somewhat greater than $1/\pi$. However, the objective here is to investigate the effects of exchange, and then in a separate paper we shall deal with an appropriate procedure for taking correlation energy into account.

In the spirit of the local-density method, the Fermi energy at point r is written, according to Eq. (6), in the form

$$E_F(r)=\tfrac{1}{2}k_F^2(r)-\frac{1}{\pi}k_F(r) . \tag{7}$$

Equations (5) and (7) combine to yield a quadratic equation for the determination of $k_F(r)$ in terms of the potential $V(r)$ and some constants. Namely,

$$k_F^2(r)-2^{3/2}\gamma k_F(r)-2[E_F+V(R)-V(r)]=0 , \tag{8}$$

where γ is an abbreviation for $1/2^{1/2}\pi$. Only the positive square-root solution of Eq. (8) is retained, as this is the choice of physical importance. Therefore

$$k_F(r)=2^{1/2}\{\gamma+[\gamma^2+E_F+V(R)-V(r)]^{1/2}\} . \tag{9}$$

The TF version of this expression is obtained in the limit $\gamma=0$. Equation (9) provides physically acceptable values of the local electron density $n(r)$ of Eq. (4). For negative values of Z, the potential becomes infinitely positive as the origin is approached. An examination of Eq. (9) shows that this behavior causes difficulty with the requirement that $k_F(r)$ be real and positive. Unphysical values of $k_F(r)$ are removed from the theory by a Coulomb hole,[21] a spherical region about the negative point-charge impurity in which the electron density vanishes, leaving only the uniform background positive charge. It is useful to keep in mind that Eq. (6) may be rewritten, for convenience, as

$$k_F=2^{1/2}[\gamma+(\gamma^2+E_F)^{1/2}] . \tag{10}$$

Self-consistency requires that the screened impurity potential satisfy Poisson's equation with a charge distribution given in terms of the screening charge density. It follows that

$$-\nabla^2 V(r)=4\pi[n(r)-n] . \tag{11}$$

The displaced electron charge density on the right-hand side of Eq. (11) is expressed in terms of $V(r)$, the ambient Fermi energy E_F, the exchange constant γ, and the constant $V(R)$ by making use of Eqs. (1), (4), (9), and (10). Equation (11) then becomes the basic nonlinear TFD equation

$$\nabla^2 V(r)=(2^{7/2}/3\pi)([\gamma+(\gamma^2+E_F)^{1/2}]^3-\{\gamma+[\gamma^2+E_F+V(R)-V(r)]^{1/2}\}^3),\quad r\leq R . \tag{12}$$

In addition to developing numerical solutions of Eq. (12) for both positive and negative integral values of Z, it is of interest to consider its linearization by assuming that it is legitimate to use a perturbation approach. This entails a binomial expansion in which the square of $[V(R)-V(r)]/(\gamma^2+E_F)$ can be neglected in comparison with unity. In that case, Eq. (12) takes on the linearized form

$$\nabla^2 V(r)=q^2[V(r)-V(R)] . \tag{13}$$

The quantity q is given by

$$q=q_0[k_F/(k_F-2^{1/2}\gamma)]^{1/2} , \tag{14}$$

where $q_0=(4k_F/\pi)^{1/2}$. In this paper zero subscripts label TF quantities.

Equations (12) and (13) first appeared in the literature about 33 years ago in connection with the problem of ionization of hydrogen in metals.[22] In that case, the impurity proton is screened by conduction electrons. When $\gamma=0$, these equations reduce to earlier ones developed by Mott,[23] who treated the screened Coulomb field in a metal neglecting exchange effects. As a description of linear screening in metals, Eq. (13) has the solution $V(R)=0$, and

$$V(r)=v(r)e^{-qr} , \tag{15}$$

which includes the boundary condition that $V(r)$ approach $v(r)$ as $r\rightarrow 0$, and is consistent with complete screening of the point charge at $r=\infty$. This implies that R is infinite for this situation. Later work[24] established numerical solutions of the nonlinear TFD equation for the screened potential around a divalent impurity in a monovalent metal. In essence, these calculations show that the linearized TF approximation, the nonlinear TF theory, and the nonlinear TFD theory lead progressively to more effectively screened impurity potentials. Insofar as linear screening effects are concerned, this trend follows at once from Eqs. (14) and (15).

III. ANALYTICAL SOLUTION OF THE LINEARIZED TFD SCREENING EQUATION

This section is concerned with linear dielectric screening effects in the homogeneous and isotropic model semiconductor. Unlike the situation for an impurity point charge in a metallic medium, the displaced electron charge density now has a finite radius R. The analysis is simplified here by dealing exclusively with positive values of Z. This restriction is removed in Sec. IV where nonlinear dielectric screening effects are considered.

Evaluation of Eq. (9) at $r=R$ leads to $k_F(R)=k_F$. Then, from Eqs. (1) and (4), it follows that $n(R)=n$, in agreement with the definition of R. For $r\geq R$, the screened potential has the form shown in Eq. (3), while in the range $r\leq R$ the solution of Eq. (13), with continuity at $r=R$, is

$$V(r)=\frac{v(r)\sinh[q(R-r)]}{\sinh(qR)}+V(R) . \tag{16}$$

Continuity of the electric field at $r=R$ provides the transcendental equation

$$\sinh(qR)=qR\epsilon(0) \tag{17}$$

for the determination of R as a function of the semiconductor parameters k_F and $\epsilon(0)$. In the metallic limit, Eq. (17) predicts $R=\infty$, a result consistent with Eq. (15). These various features of the linearized TFD description of impurity screening in metals and semiconductors are familiar from the TF theory.[1]

An expression for the TFD spatial dielectric function follows from Eqs. (2) and (16). Again, the result is a replica of the Z-independent TF form given by

$$\tilde{\epsilon}(r)=\begin{cases}\epsilon(0)qR/\{\sinh[q(R-r)]+qr\}, & r\leq R\\ \epsilon(0), \quad r\geq R .\end{cases} \tag{18}$$

Numerical illustrations of Eq. (18) for diamond, Si, and Ge are displayed in the next section. It will be seen that $\tilde{\epsilon}(r)$ exceeds the same TF spatial dielectric function over the range $0<r<R$. Thus, it follows from these calculations that the impurity potential is more effectively screened when exchange effects are included in the valence-electron gas of the host semiconductor, a behavior already known[22] from the metallic case and traced to the reduced probability of two electrons with parallel spins approaching one another closely. This effect, due to the exclusion principle, lowers the energy of the system.

The linear-response wave-vector-dependent dielectric function is defined as the ratio $\tilde{v}(k)/\tilde{V}(k)$, where $\tilde{v}(k)$ and $\tilde{V}(k)$ are the Fourier transforms of the unscreened and screened potentials, respectively. In the present case, this prescription yields

$$\epsilon(k)=\frac{q^2+k^2}{k^2+[q^2\sin(kR)/\epsilon(0)kR]} . \tag{19}$$

For a given semiconductor, the TFD-model dielectric functions require characteristic value of q and R obtained from Eqs. (14) and (17) in terms of the static macroscopic

TABLE I. Listing of physical parameters and characteristic quantities entering in the linearized TF and TFD models of dielectric screening for diamond, Si, and Ge.

	Diamond	Silicon	Germanium
Nearest-neighbor distance a (a.u.)	2.91	4.44	4.63
Static dielectric constant $\epsilon(0)$	5.7	11.94	16.0
Valence Fermi momentum k_F (a.u.)	1.46	0.96	0.98
E_{0F} (a.u.)	1.06	0.46	0.48
E_F (a.u.)	0.60	0.16	0.17
$q_0=(4\pi/k_F)^{1/2}$	1.36	1.10	1.12
$q=q_0[k_F/(k_F-2^{1/2}\gamma)]^{1/2}$	1.54	1.35	1.36
Screening radius R_0 (a.u.)	2.76	4.28	4.54
Screening radius R (a.u.)	2.44	3.50	3.74

dielectric constant $\epsilon(0)$ and the valence Fermi momentum k_F. Clearly, the TF-model dielectric functions $\bar{\epsilon}_0(r)$ and $\epsilon_0(k)$ are recovered when $\gamma=0$.

IV. LINEAR TFD DIELECTRIC FUNCTIONS FOR DIAMOND, SILICON, AND GERMANIUM

The static macroscopic dielectric constant $\epsilon(0)$ and the valence Fermi momentum k_F for diamond, Si, and Ge are listed in Table I. For reasons given in Ref. 3, the effective number of valence electrons per atom used in calculating k_F for Ge is 5, while for diamond and Si the number is 4. The Fermi energy E_F, the screening radius R, and the quantity q, along with their TF counterparts, for each of the semiconductors, are also included in the listing. The TFD and TF wave-vector-dependent dielectric functions for diamond, Si, and Ge are calculated from Eq. (19) and illustrated in Fig. 1. The spatial dielectric functions are

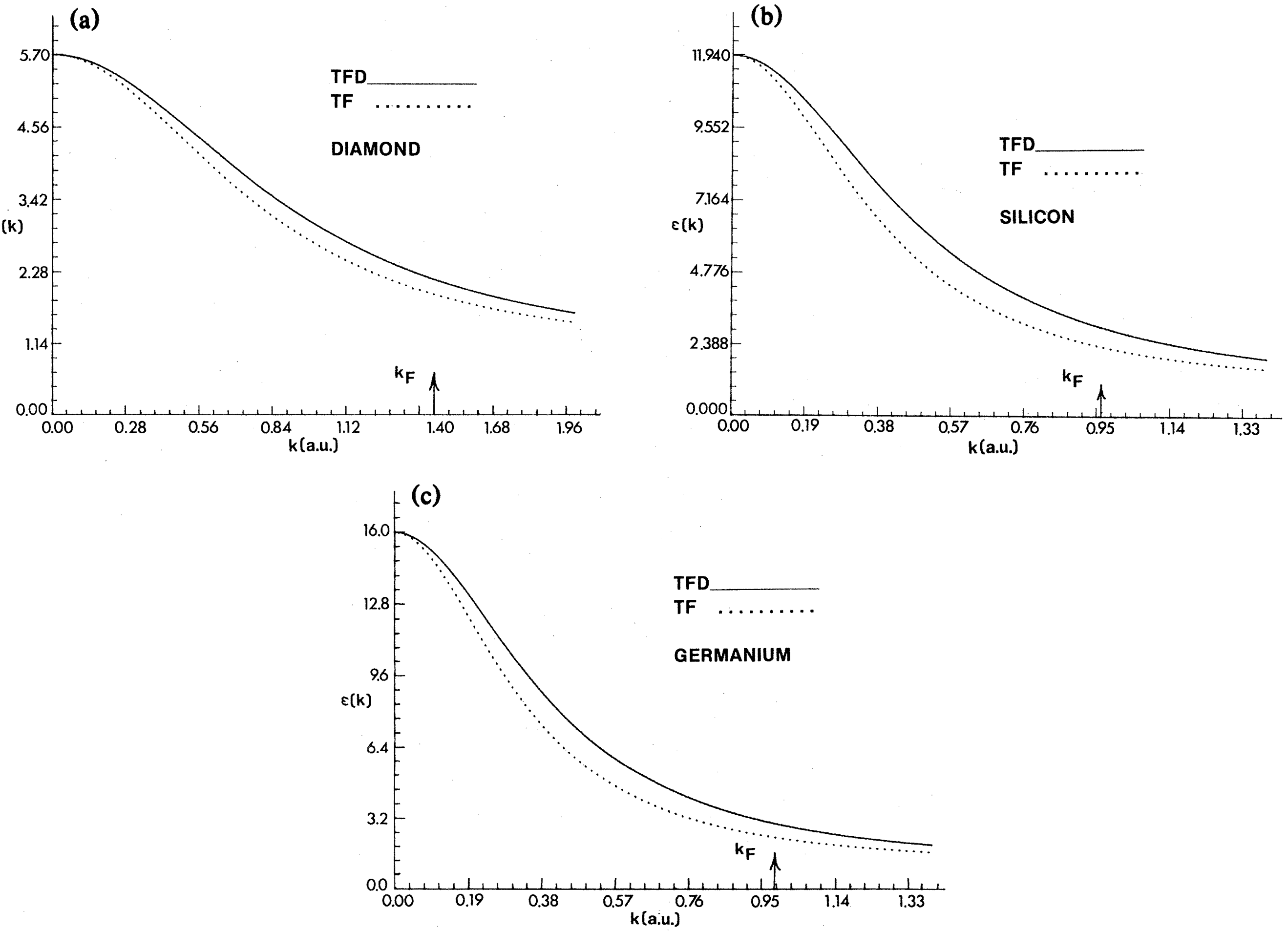

FIG. 1. TF and TFD wave-vector-dependent dielectric functions for diamond, silicon, and germanium in the linear regime.

obtained from Eq. (18) and displayed in Fig. 2.

A comparison between the TF and Srinivasan's Penn-model wave-vector-dependent dielectric functions has been given in Ref. 1. Except for the low-k region, TF predictions are consistently on the high side of a close numerical match with Srinivasan's calculations. The small-k behavior[13] of the right-hand side of Eq. (19) is a quadratically decreasing function of k with no peak similar to that appearing in Srinivasan's results. Moreover, the TF results are surprisingly close to the same functions calculated on the basis of accurate band structure for Si and Ge along the [100] direction. These quantitative agreements are particularly impressive in view of the analytical simplicity of $\epsilon_0(k)$. An even simpler analytical fit to the accurate $\vec{k}$-theory calculations of Ref. 2 is available.[16] However, an arbitrary constant in this expression was devoid of physical significance until a comparison[13] with $\epsilon_0(k)$ was made at low k.

While Srinivasan has emphasized that a spatial dielectric function should attain its limiting value over a distance of the order of the nearest-neighbor distance, his function overshoots $\epsilon(0)$. On the other hand, $\bar{\epsilon}_0(r)$ shows a smooth monotonic approach to $\epsilon(0)$ with no such overshoot. A comparison of the two cases for diamond, Si, and Ge is made in Ref. 1, where it is seen that $\bar{\epsilon}_0(r)$ is in close agreement with Penn-model results.

Figure 1 shows that $\epsilon(k)$ and $\epsilon_0(k)$ are monotonically decreasing functions of k, a behavior also characteristic of the accurate band-structure calculation mentioned above. In light of the comparisons made in Ref. 1, and in view of Fig. 1, it is evident that $\epsilon_0(k)$ is more closely representative of the linear-response functions of Walter and Cohen for real materials. With regard to the spatial dielectric functions, Fig. 2 makes it clear that $\bar{\epsilon}(r)$ and $\bar{\epsilon}_0(r)$ are smooth monotonic functions of r, while the former attains the limiting value $\epsilon(0)$ before the latter. Thus, as already noted, $V(r)$ is more effectively screened than $V_0(r)$. The inclusion of exchange energy in the TF theory is conceptually in the right direction for improvement, however, it acts to diminish the accuracy of the TF dielectric functions $\bar{\epsilon}_0(r)$ and $\epsilon_0(k)$.

It is of interest to examine the range of validity of the linearized TFD screening equation. As before, consider Z positive. This approximation involves a binomial expansion in which the square of $[V(R)-V(r)]/(\gamma^2+E_F)$ is neglected in comparison with unity, or equivalently,

$$\frac{Z}{r}\frac{\sinh[q(R-r)]}{\sinh(qR)}<E_F+\gamma^2\ , \tag{20}$$

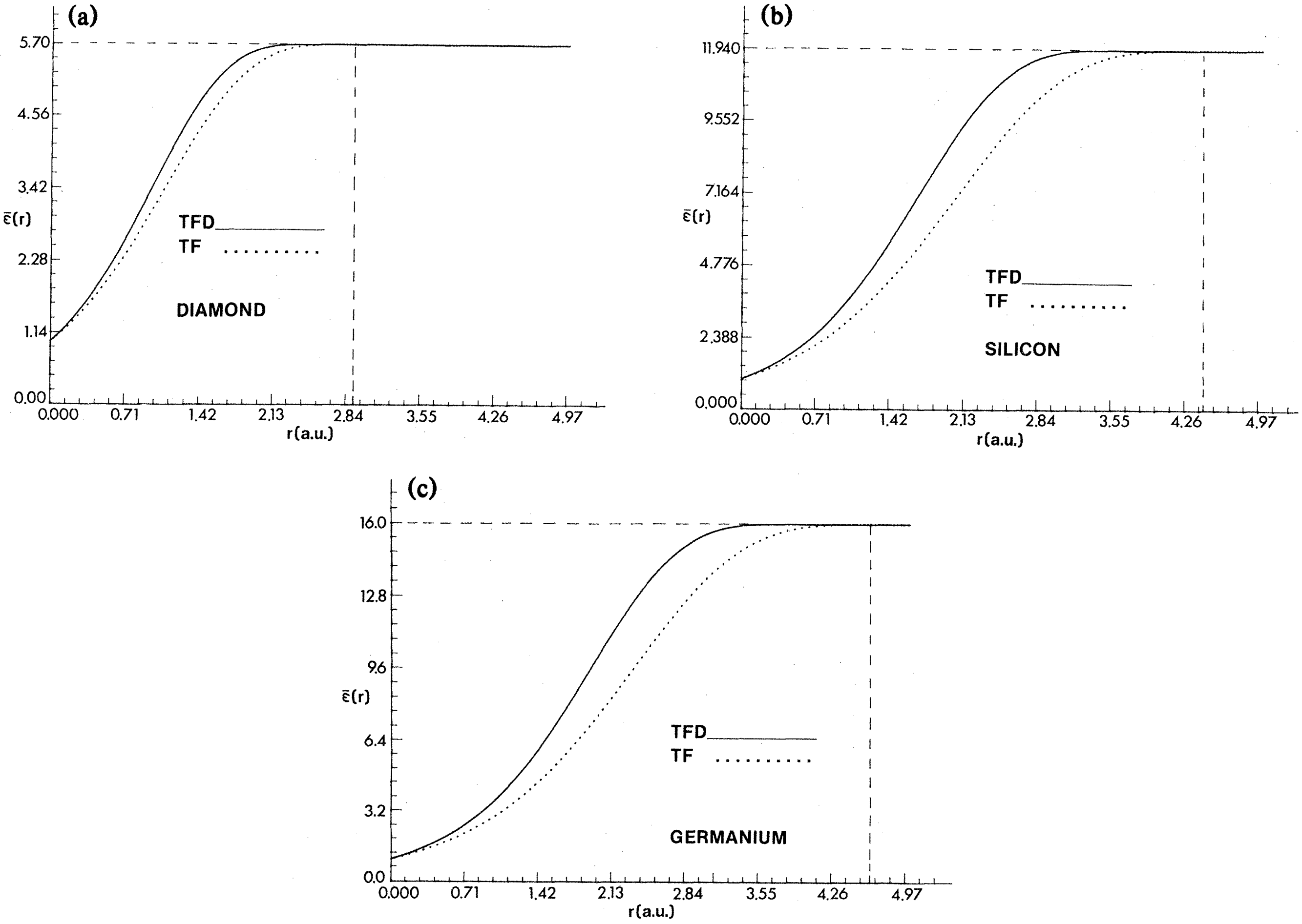

FIG. 2. TF and TFD spatial dielectric functions for diamond, silicon, and germanium in the linear regime. In each case the single bond length is denoted by the vertical (dashed) line.

TABLE II. Listing of various measures of the range of validity of the linearized TF and TFD screening equations for diamond, Si, and Ge when $Z=1$. TF values are in parentheses.

	Diamond	Silicon	Germanium
r_1 (a.u.)	0.60(0.49)	1.09(0.85)	1.06(0.83)
r_1/a	0.21(0.17)	0.24(0.19)	0.23(0.18)
r_1/R	0.25(0.18)	0.31(0.20)	0.28(0.18)
$\bar{\epsilon}(r_1)$	2.29(1.84)	3.92(2.46)	3.98(2.47)
$[\bar{\epsilon}(r_1)/\epsilon(0)](100\%)$	40.2(32.3)	32.8(20.6)	24.9(15.4)

where Eq. (16) is used in arriving at Eq. (20). This inequality does not hold for all values of r between the origin and R. When $Z=1$, it does not hold and neither does the linear approximation, for values of r less than a critical value r_1 given in Table II for diamond, Si, and Ge. The inequality in Eq. (20) becomes an equality at $r=r_1$. The meaning of r_1 is visualized by comparing it with the nearest-neighbor distance a and the screening radius R. Rows 2 and 3 in Table II list the ratios of r_1 and these lengths, respectively. Further insight is gained by evaluating the spatial dielectric function at r_1, and then determining the percentage of the static macroscopic constant $\epsilon(0)$ attained at $r=r_1$. These quantities are given in rows 5 and 6 of Table II. These various comparisons and analogous ones in the linearized TF theory[25] show for each semiconductor that (1) r_1 is greater than r_0, making the former even more meaningful than the latter on the lattice scale, (2) the fraction (roughly $\frac{1}{4}$) of the screening radius over which the linearized TFD equation is invalid exceeds the already significant TF fraction (about $\frac{1}{5}$), and (3) on the order of 10% more of $\epsilon(0)$ is reached at $r=r_1$ than at $r=r_0$. From these results, it is clear that the TFD theory is less tolerant of linearization than the TF scheme. The space region about the impurity in which this approximation is meaningless is larger in the former. In either case, the assumption underlying the perturbation approach is destined to fail since it certainly is not correct very close to the impurity where $-V$ approaches infinity.

Another point of interest here concerns the trend in the above results when Z is increased. To examine this aspect, the previous calculations and comparisons are repeated for a doubly charged donor ion. The numerical results are presented in Table III where r_2 is the new value of the independent variable below which the linearized TFD screening equation fails. From the increase in r_2 over r_1, it is seen that the breakdown region has grown from roughly $\frac{1}{4}$ to $\frac{1}{3}$ of the screening radius. In the TF case the corresponding charge is from about $\frac{1}{5}$ to $\frac{1}{4}$. Moreover, each of the various other measures in Table III shows an increase from its value in Table II.

Clearly, the linear form of the TFD screening equation is less successful than its TF equivalent, and in both cases perturbation theory is less useful, the larger the attractive point charge Z. The latter conclusion has already been pointed out in the TF context,[25] and is consistent with the sizable deviations from linear behavior seen in the nonlinear dielectric functions for large values of Z. A striking donor-acceptor asymmetry found in these deviations is even more prominent in the nonlinear TFD-model dielectric functions presented in the following section. Within the restrictions of the law governing the process of linearization, it is known[26] that the approximation is exact only for vanishingly small impurity charges. It is not surprising, therefore, to find trouble rooted in Eq. (16), which is only valid in the mathematical limit $Z\rightarrow 0$.

V. NONLINEAR TFD SCREENING THEORY FOR POSITIVE AND NEGATIVE IMPURITY IONS

The purpose of this section is to present the TFD theory of nonlinear impurity screening for different point charges in the model semiconductor. The self-consistent screened potential around an impurity donor or acceptor ion in diamond, Si, or Ge is obtained by numerical solution of an appropriate set of linear and nonlinear equations. For positive values of Z, the potential satisfies Eq. (12) and Laplace's equation for $r\leq R$ and $r\geq R$, respectively. The desirable solution of these equations approaches $v(r)/\epsilon(0)$ and $v(r)$ as r approaches infinity and the origin, respectively. Moreover, the potential and the electric field are continuous at $r=R$.

As noted previously, negative values of Z require a different treatment due to the Coulomb hole surrounding the point charge. No electrons are allowed in this region of negative kinetic energy, and hence the range of validity of the nonlinear TFD screening equation is subject to the constraint

$$V(r)\leq E_F+\gamma^2+V(R)\ . \tag{21}$$

TABLE III. Listing of various measures of the range of validity of the linearized TF and TFD screening equations for diamond, Si, and Ge when $Z=2$. TF values are in parentheses.

	Diamond	Silicon	Germanium
r_2 (a.u.)	0.84(0.71)	1.41(1.18)	1.38(1.15)
r_2/a	0.29(0.24)	0.32(0.27)	0.30(0.25)
r_2/R	0.34(0.26)	0.40(0.28)	0.37(0.25)
$\bar{\epsilon}(r_2)$	3.00(2.37)	5.49(3.41)	5.73(3.45)
$[\bar{\epsilon}(r_2)/\epsilon(0)](100\%)$	52.6(41.6)	46.0(28.6)	35.8(21.5)

TABLE IV. Listing of screening radii and Coulomb-hole radii for nonlinear TFD screening equation for diamond, Si, and Ge when $Z=\pm 1$, ± 2, ± 3, and ± 4. TF values of Ref. 3 are in parentheses, and $Z=0$ corresponds to the linear results of Table I.

	Z	Diamond	Silicon	Germanium
Screening radius R (a.u.)	4	2.18(2.44)	3.11(3.74)	3.37(4.02)
	3	2.22	3.17	3.43
	2	2.27	3.24	3.50
	1	2.34(2.64)	3.34(4.06)	3.60(4.33)
	0	2.44(2.76)	3.50(4.28)	3.74(4.54)
	−1	2.72(2.93)	4.29(4.63)	4.48(4.86)
	−2	2.95	4.83	5.00
	−3	3.14	5.25	5.40
	−4	3.31(3.30)	5.61(5.28)	5.74(5.47)
Coulomb-hole radius R_c (a.u.)	−1	0.70(0.53)	1.50(0.97)	1.44(0.93)
	−2	1.06	2.18	2.11
	−3	1.33	2.69	2.59
	−4	1.54(1.21)	3.11(2.06)	3.00(1.98)

The radius R_c of the Coulomb hole is defined by the equality in Eq. (21). In this case, Eq. (12) is restricted to the region between R and R_c, while the Poisson's equation,

$$\nabla^2 V(r)=(2^{7/2}/3\pi)E_F^{3/2}\ , \tag{22}$$

describes the solution inside the hole. Here, the potential and its derivative are continuous at $r=R$ and $r=R_c$. A detailed discussion of Eq. (22), in the TF framework, has been given in Refs. 21 and 3 for metals and semiconductors, respectively. As a result, the potential inside the

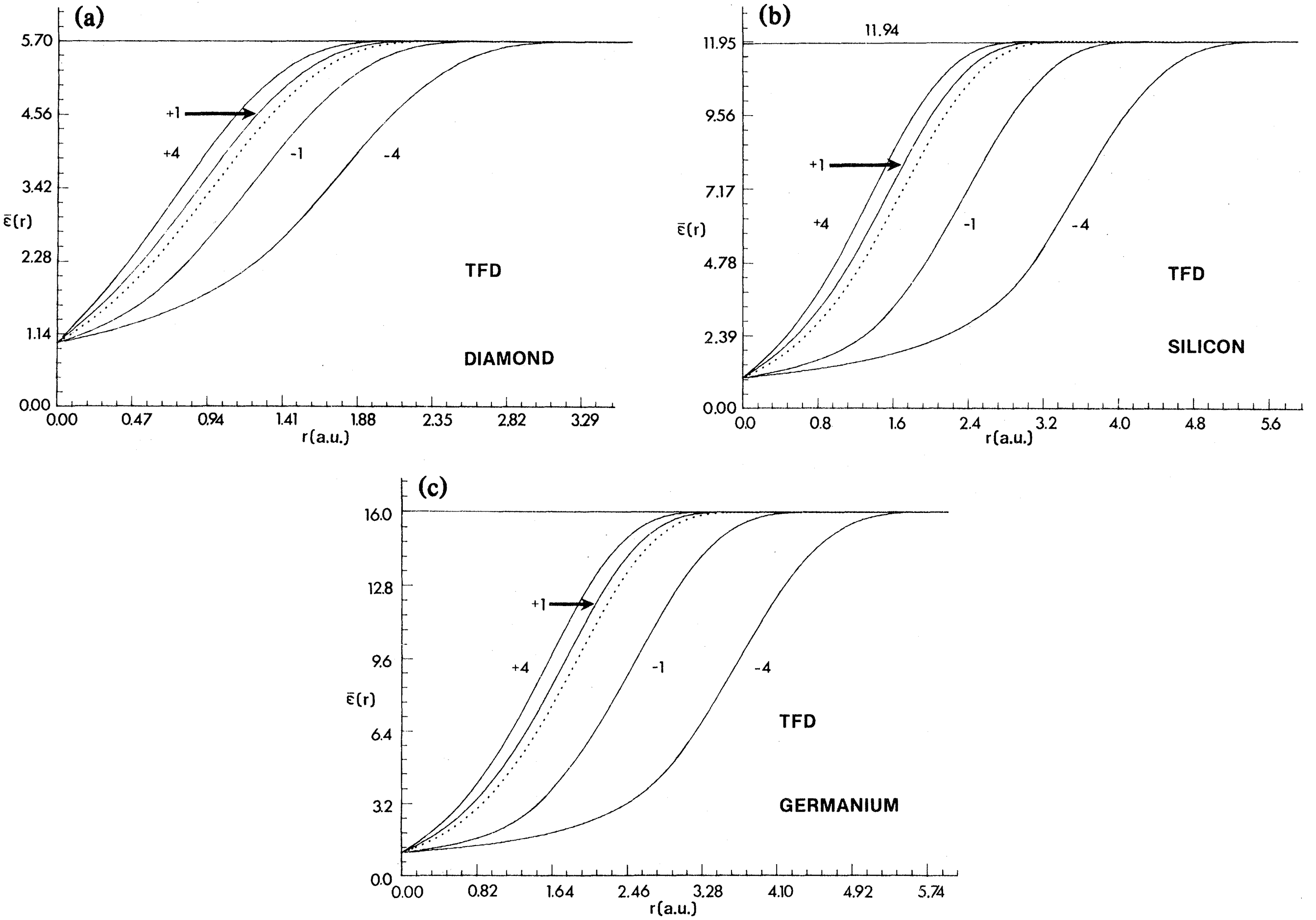

FIG. 3. TFD spatial dielectric functions for diamond, silicon, and germanium in the nonlinear regime when $Z=\pm 1$ and ± 4. The dotted line denotes the Z-independent linear regime.

sphere is known to be

$$V(r)=v(r)+(2^{5/2}/9\pi)E_F^{3/2}r^2+\beta\ , \tag{23}$$

where the unknown constant β is determined by the continuity of the potential at $r=R_c$. It should be noted that E_F appearing in Eqs. (22) and (23) is given by Eq. (6).

The mathematical problems encountered here are essentially the same as those described in Ref. 3 for positive and negative values of Z. The nonlinear TFD screening equation with initial conditions is solved in terms of the numerical strategy outlined there in the TF context. The actual numerical calculations were carried out with the use of a Runge-Kutta-Verner fifth- and sixth-order method.[27] The matching of dependent variables to satisfy correct behavior at the origin or continuity at $r=R_c$ was rigorously established to within 10^{-3}. In order to solve the nonlinear TF problem, it is only necessary to set $\gamma=0$ in the input data file of the computer program for the TFD case. TF results checked in this manner were found to be in excellent agreement with values of the screening radii and Coulomb-hole radii presented in Ref. 3, where use was made of a modified predictor-corrector numerical method of solution.

VI. NONLINEAR TFD DIELECTRIC FUNCTIONS FOR DIAMOND, SILICON, AND GERMANIUM

Table IV reports the screening radii R and the Coulomb-hole radii R_c for diamond, Si, and Ge obtained from the numerical solution of the nonlinear TFD impurity screening problem defined in the preceding section. Results are given for monovalent, divalent, trivalent, and tetravalent donor and acceptor substitutional ions. For comparison, screening radii and Coulomb-hole radii relevant to the nonlinear TF problem solved in Ref. 3, for the monovalent, and tetravalent cases, are also listed in parentheses. Moreover, linear results from Table I are included and denoted as $Z=0$.

In the spirit of Eq. (2), nonlinear spatial dielectric functions can be found from the numerical impurity potentials derived in the search for the screening radii and Coulomb-hole radii. The results are illustrated in Fig. 3, where the dotted curves represent the linear ($Z=0$) approximation. For simplicity of presentation, the spatial dielectric functions characteristic of the divalent and trivalent cases are not included in these figures. General features of these curves are familiar from the TF model. For each semiconductor, the results for positive and nega-

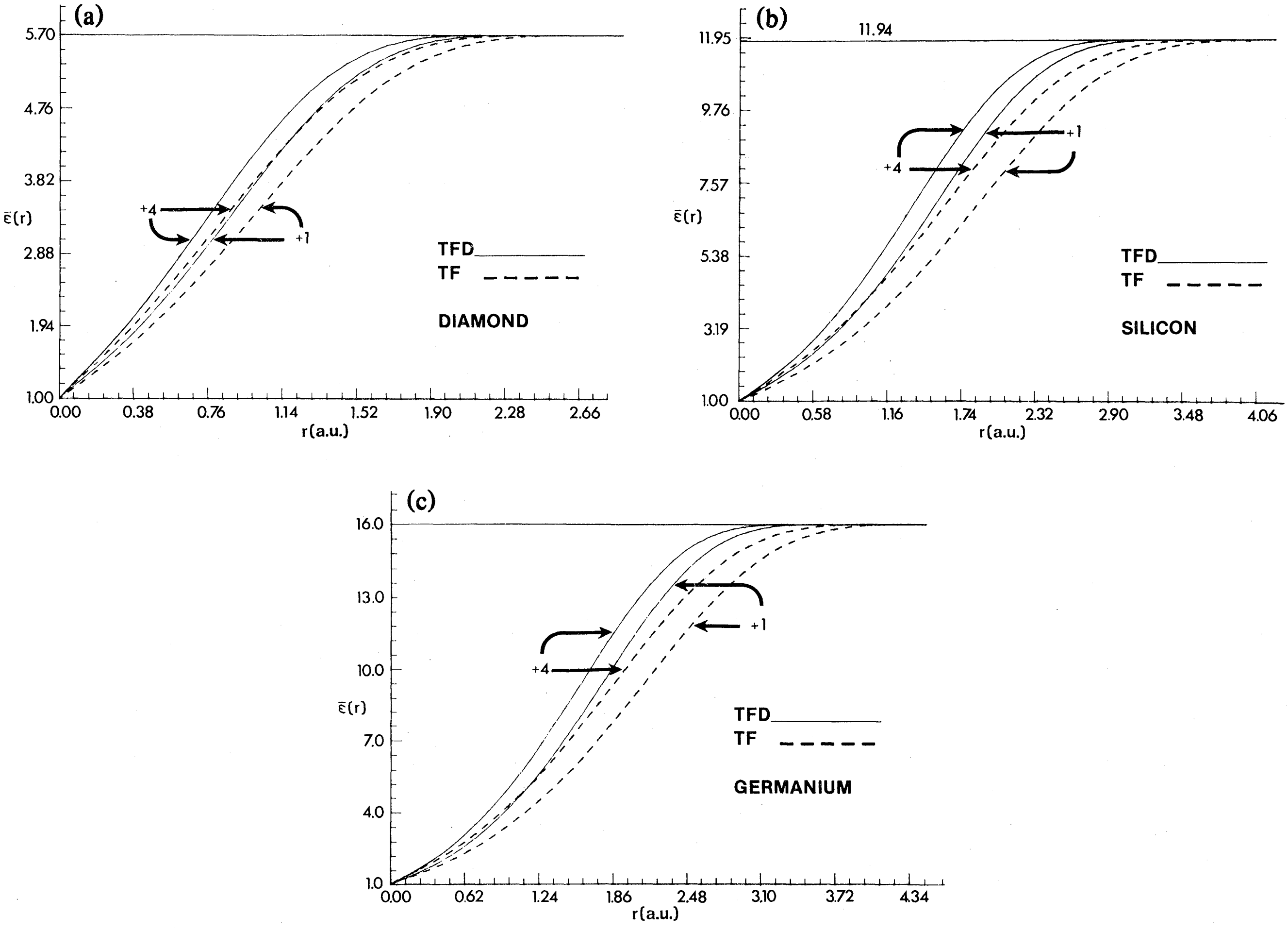

FIG. 4. Comparison of the TF and TFD spatial dielectric functions in the nonlinear regime for diamond, silicon, and germanium when $Z=+1$ and $+4$.

tive ions fall above and below the linear curve, respectively. Thus, nonlinear screening tends to reduce attractive potentials and enhance repulsive potentials. Corrections to linear-response theory are substantial, especially in the latter case. Moreover, ion-charge conjugation leads to unsymmetrical shifts in the curves.

It is of interest to compare nonlinear-response functions in the two models. In the TF scheme, spatial dielectric functions are based on the screening radii and Coulomb-hole radii given in Table IV (the numbers in parentheses). For monovalent and tetravalent donors, Fig. 4 consistently shows that effects of nonlinearity and exchange are more effective at reducing attractive potentials than the former acting alone. Alternatively, there are situations in which nonlinearity alone more capably enhances an attractive potential, as shown by the monovalent cases in Fig. 5. Tetravalent acceptor potentials are seen to be consistently more enhanced by the presence of both effects. It also appears that donor-acceptor asymmetry is even stronger in the TFD theory. Judged from these figures, exchange introduces important differences between the TF and TFD descriptions of nonlinear dielectric screening.

VII. CONCLUDING REMARKS

In the linear regime, the TFD theory of screening in semiconductors is deficient as an approximate description of dielectric functions when compared with the TF theory and exact band-structure calculations for Si and Ge. This outcome is not entirely surprising since the TFD approach has various shortcomings. From the outset, it carries no form of dynamical correlation between the electrons of opposite spin. For this reason alone, the TFD model cannot be expected to yield good results within the degenerate-electron-gas framework. Thus, as noted earlier, the inclusion of correlation[28] is presumably the next natural step toward improving the TFD-model dielectric functions.

More generally, if the TF theory is regarded as the first approximation of a systematic expansion in powers of Planck's constant, then the next term allows for the exchange energy and for a gradient quantum correction[29] to the TF form of the kinetic energy. From this viewpoint, another direction for improving the TFD dielectric functions involves taking account of the quantum correction.[30]

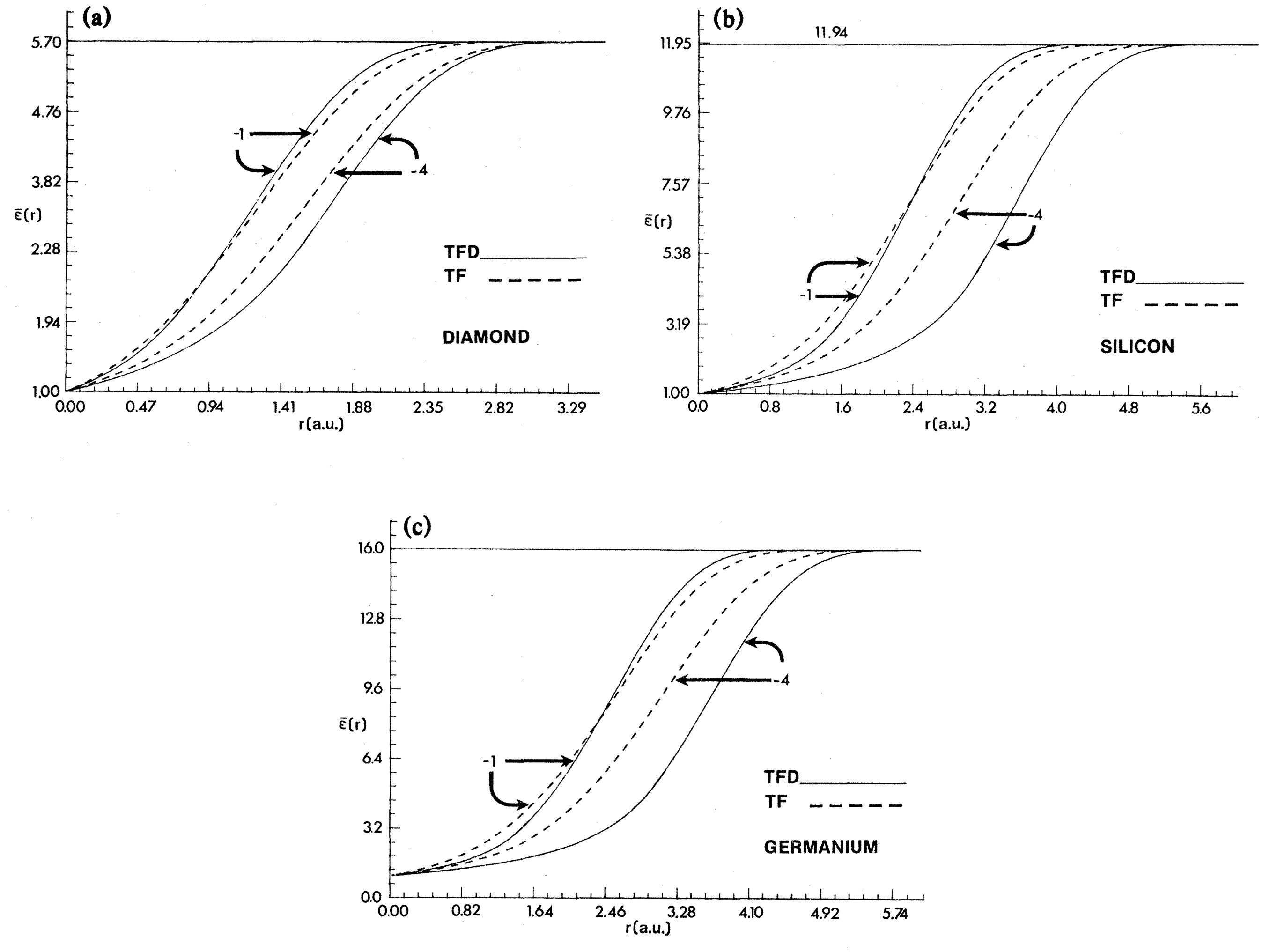

FIG. 5. Comparison of the TF and TFD spatial dielectric functions in the nonlinear regime for diamond, silicon, and germanium when $Z=-1$ and -4.

The TF theory itself neglects exchange, correlation, and the quantum correction, and yet it still provides very respectable linear-response functions for real semiconductors. This suggests that adding correlation energy and/or the quantum correction to the TFD theory will be useful if the result is to reduce the effects of exchange and further improve the behavior of the statistical model of dielectric screening. These extentions of the TFD theory are presently under investigation.

Note added in proof. After completion of this work, it was learned that the linearized TFD theory has been discussed by P. Csavinszky [Phys. Rev. B 28, 6076 (1983)]. Although the spirit of his approach is close to that which leads to Eqs. (13) and (14) of this paper, there is a significant difference in the choice of the quantity in terms of which the linearization is implemented.

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