

Exchange correlation in the $X\alpha$ approximation and shallow-donor impurity ionization energy

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The Thomas-Fermi-Dirac (TFD) theory of dispersive valence screening of an ionized impurity in a semiconductor is extended to include exchange correlation in the $X\alpha$ approximation. Linearization of the resulting screening equation yields a closed analytical expression for the spatial dielectric function of the electron-gas model semiconductor. The exchange-correlation potential of a shallow-donor impurity and the exchange interaction of the donor electron with the valence electrons are used in an effective-mass, three-parameter, variational calculation of the donor ionization energy. A single-band model and electronic constants appropriate to silicon are used for illustration. Marked differences are noted between the results of this application of linearized TFD screening and those reported previously by another author, who calculated the ionization energy on the basis of an incomplete formulation of the basic nonlinear screening equation in the $X\alpha$ approximation.

I. INTRODUCTION

The response of the valence electrons of an undoped semiconductor to a static substitutional point-charge impurity Z has been described in terms of the Thomas-Fermi (TF) screening theory,^{1,2} and its Thomas-Fermi-Dirac (TFD) refinement including exchange.^{3,4} The latter method has been extended⁵ to account for correlation within the framework of the Dirac-Slater local-density treatment of exchange by means of the $X\alpha$ approximation.⁶ In the uniform-electron-gas model,⁷ the Fermi energy E_F consists of the kinetic energy $k_F^2/2$, the pure exchange energy $-k_F/\pi$, and the correlation energy $E_c(k_F)$, where k_F is the maximum electron momentum. A practical way to simulate electron exchange correlation is to ignore $E_c(k_F)$ and multiply the pure exchange term by the factor $3\alpha/2$, where α is a parameter with values ranging from 1 to $\frac{2}{3}$. In the local-density scheme, $\alpha=1$ gives the Slater⁶ exchange potential, while $\alpha=\frac{2}{3}$ corresponds to the exchange potential first derived by Dirac⁸ and rederived by Gáspár⁹ and by Kohn and Sham.¹⁰ The importance of including the exchange-correlation potential in the Hamiltonian for the valence electrons is well known from self-consistent pseudopotential band calculations in silicon.¹¹

Dielectric relaxation of the host semiconductor is conveniently characterized by the spatial dielectric function $\bar{\epsilon}(r)$ defined as the ratio of the bare Coulomb potential, $-Z/r$, to the screened potential, $V(r)$. The TFD equation for the screened potential has been solved analytically and numerically in the linear and nonlinear regimes, respectively.¹² Spatial dielectric functions, screening radii, and Coulomb-hole radii, with exchange-correlation potential strength α and ion charge state Z as parameters, have been plotted and tabulated.¹² A variational principle equivalent of the basic nonlinear TFD screening equation yields approximate analytical dielectric functions, screening radii, and Coulomb-hole radii that show

very good agreement with the exact numerical results.¹² In recent literature,¹³ the TF and TFD (pure exchange only) screening theories have been applied to donor and acceptor impurities in the compound semiconductors GaAs and GaP. These applications have also been studied independently in Ref. 12 in the $X\alpha$ approximation. Results obtained in Ref. 12 for position- and momentum-space dielectric functions, screening radii, and Coulomb-hole radii for $\alpha=0.0$ and 0.67 are in excellent agreement with those presented in Ref. 13.

One of the many applications of the spatial dielectric function is the calculation of the ionization energy of a screened impurity (donor) electron. A consistent treatment of this problem must incorporate the exchange-correlation interaction of the donor electron with the valence electrons. Such a calculation has been presented in Ref. 5. However, it is based on the incomplete formulation of the TFD screening theory given in Ref. 3. Here, we extend the TFD screening theory of Ref. 4 to include exchange-correlation effects in the $X\alpha$ approximation and carry out a fully consistent variational calculation of the shallow-donor ionization energy using the linearized TFD dielectric screening function.

Section II reviews the TFD method and an equivalent variational principle in the $X\alpha$ approximation for a system of valence electrons. Minimization of the total ground-state energy with respect to the electron number density $n(r)$, subject to the constraint that the total number of electrons is constant, leads to a nonlinear relationship between $n(r)$ and $V(r)$. Self-consistency requires that the screened potential satisfy Poisson's equation with charge density $n(r)$ displaced by the uniform background electron density n . The resulting TFD equation is linearized under the assumption that a perturbation approach is valid, and then solved in closed form for the point-charge screened potential. Section III is concerned with a three-parameter variational calculation of shallow-donor ionization energy including the linearized

exchange-correlation potential and the exchange interaction of the donor electron with the valence electrons. For this purpose, the semiconductor is described by a single conduction band with one minimum and electronic constants appropriate to silicon are used. The variational calculation is implemented for various core charges Z and exchange-correlation strengths α . In Sec. IV, results for donor ionization energies are given in tabular and graphical forms. Marked differences between these results and those reported in Ref. 5 are noted. 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) and mass (m), and \hbar are set equal to unity.

II. TFD METHOD IN THE $X\alpha$ APPROXIMATION AND AN EQUIVALENT VARIATIONAL PRINCIPLE

As mentioned above, the Fermi energy of the uniform valence-electron gas, including the effect of exchange correlation in the $X\alpha$ approximation, is written as the sum of two terms,

$$E_F = \frac{k_F^2}{2} - \frac{3\alpha}{2\pi} k_F. \quad (1)$$

The maximum or Fermi momentum k_F is expressed in terms of the uniform electron density n by

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

Correlation energy between electrons of parallel spins increases the numerical coefficient of k_F to a value somewhat greater than its pure exchange value $1/\pi$. In the local-density approximation, Eq. (2) is applied to an inhomogeneous electron gas with $n(r)$ as the nonuniform electron density at point r . If $k_F(r)$ denotes the corresponding Fermi momentum, then by Eq. (1) the local Fermi energy is expressed as

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

The assumption of no electron redistribution is embodied in the equilibrium condition

$$E_F(r) + V(r) = E_F + V(R), \quad (4)$$

where E_F is the r -independent ambient Fermi energy (chemical potential at absolute zero) and R is the finite radius of dielectric screening at which $n(r)$ becomes equal to the uniform electron density n in the absence of a perturbing impurity potential. At and beyond $r=R$, the bare Coulomb potential is screened by the macroscopic dielectric constant $\epsilon(0)$. The valence electrons are assumed to move in the common screened potential $V(r)$. Equations (3) and (4) yield a quadratic equation for $k_F(r)$, the physical solution of which leads to the electron density

$$n(r) = \frac{2^{3/2}}{3\pi^2} \left[\frac{3\alpha}{2^{3/2}\pi} + \left(\frac{9\alpha^2}{8\pi^2} + E_F + V(R) - V(r) \right)^{1/2} \right]^3. \quad (5)$$

This paper deals exclusively with positive values of Z . For negative values of Z (acceptors), the potential $V(r)$ becomes infinitely positive as r approaches the origin. Inspection of Eq. (5) shows that this behavior is inconsistent with the physical requirement that $n(r)$ be real and positive. Negative values of Z require a different treatment and will not be considered here. Equation (5) reduces to its TF form when $\alpha=0$.

A variational principle equivalent of the TFD method has been outlined in Ref. 5 following the procedure given by March.¹⁴ A brief account of this approach is included here for completeness. The total ground-state energy of the system of valence electrons is given in atomic units by

$$E = c_k \int n^{5/3}(r) d\tau + \int n(r) V_N(r) d\tau + \frac{1}{2} \int n(r) V_e(r) d\tau - \frac{3}{2} \alpha c_e \int n^{4/3}(r) d\tau, \quad (6)$$

$$c_k = \frac{3}{10} (3\pi^2)^{2/3}, \quad c_e = \frac{3}{4} \left(\frac{3}{\pi} \right)^{1/3}.$$

The nuclear potential energy created by any nuclei is denoted by $V_N(r)$, while $V_e(r)$ is the potential energy created by the electron charge cloud. The first and fourth terms on the right-hand side of Eq. (6) represent, respectively, the kinetic energy and the exchange-correlation energy. The variational principle

$$\delta(E - [E_F + V(R)]N) = 0 \quad (7)$$

is equivalent to the TFD method. The quantity $E_F + V(R)$ plays the role of a Lagrange multiplier taking care of the constraint that the total number of electrons,

$$N = \int n(r) d\tau, \quad (8)$$

is constant. Constrained minimization of the functional $E - [E_F + V(R)]N$, with respect to the local density $n(r)$, gives

$$E_F = \frac{5}{3} c_k n^{2/3}(r) + V_N(r) + V_e(r) - V(R) - 2\alpha c_e n^{1/3}(r). \quad (9)$$

It remains to identify $V_N(r) + V_e(r)$ as the total electrostatic potential $V(r)$ and to note that Eq. (9) may be reexpressed as an equation for $n(r)$ which coincides with Eq. (5).

The displacement of the inhomogeneous electron density $n(r)$ from the average unperturbed background density n provides the source term in Poisson's equation for the self-consistent screened potential $V(r)$. The uniform electron density n is recovered from Eq. (5) by setting r equal to the screening radius R . Thus,

$$n = \frac{2^{3/2}}{3\pi^2} \left[\frac{3\alpha}{2^{3/2}\pi} + \left(\frac{9\alpha^2}{8\pi^2} + E_F \right)^{1/2} \right]^3. \quad (10)$$

Note that Eq. (10) is in agreement with Eqs. (1) and (2).

Clearly, an inconsistent formulation of the screening equation in the $X\alpha$ approximation will result if this form of n does not include the exchange-correlation strength α . This is precisely the case for the screening equations in Refs. 3 and 5 which are based on the TF ($\alpha=0$) ex-

pression for E_F . This important difference between the present formulation of the TFD equation and that given in Refs. 3 and 5 originates from the incomplete expression for E_F used by these authors.

The complete set of equations for $V(r)$ are

$$\nabla^2 V(r) = \begin{cases} \frac{2^{7/2}}{3\pi} \left\{ \left[\frac{3\alpha}{2^{3/2}\pi} + \left(\frac{9\alpha^2}{8\pi^2} + E_F \right)^{1/2} \right]^3 - \left[\frac{3\alpha}{2^{3/2}\pi} + \left(\frac{9\alpha^2}{8\pi^2} + E_F + V(R) - V(r) \right)^{1/2} \right]^3 \right\}, & r \leq R \\ 0, & r \geq R \end{cases} \quad (11)$$

It will be noted that Eq. (11) is simply Eq. (12) of Ref. 4 with the pure exchange parameter γ replaced by the quantity $3\alpha/2^{3/2}\pi$. The valence Fermi energy in Eq. (11) is given by Eq. (1), as emphasized above.

The nonlinear problem posed by Eqs. (11) and (12) has been solved numerically, and, in terms of a variational principle, is equivalent.¹² These results will be reported elsewhere and will include the negative- Z case. It is of interest here to consider Eq. (11) in its linearized form. A binomial expansion of the second term on the right-hand side of Eq. (11), in which the square of the quantity

$$[V(R) - V(r)] / \left[\frac{9\alpha^2}{8\pi^2} + E_F \right]$$

is neglected in comparison with unity, leads to

$$\nabla^2 V(r) = q^2 [V(r) - V(R)] \quad (13)$$

The quantity q carries the effect of the exchange correlation and has the form

$$q = q_0 \left[k_F / \left(k_F - \frac{3\alpha}{2\pi} \right) \right]^{1/2} \quad (14)$$

If exchange correlation is neglected ($\alpha=0$), q reduces to the TF screening length q_0 given by

$$q_0 = (4k_F/\pi)^{1/2}, \quad (15)$$

as expected. For $r \geq R$, the potential $V(r)$ has the Coulomb form screened by $\epsilon(0)$. In the range $r \leq R$, the solution of Eq. (13) for a point-charge external disturbance is

$$V(r) = -\frac{z}{\bar{\epsilon}(r)r}, \quad (16)$$

$$\bar{\epsilon}(r) = \begin{cases} \frac{\epsilon(0)qR}{\sinh[q(R-r)] + qr}, & r \leq R \\ \epsilon(0), & r \geq R, \end{cases} \quad (17a)$$

$$(17b)$$

$$\sinh(qR) = \epsilon(0)qR \quad (18)$$

Equation (18) follows from continuity of the electric field

at $r=R$. Input parameters for the determination of the spatial dielectric function and the screening radius, for a given semiconductor, are the static macroscopic dielectric constant, the valence Fermi momentum, and the exchange-correlation strength.

Expressed as a power series in the exchange-correlation strength, q^2 has the form

$$q^2 = q_0^2 + \sum_{l=1}^{\infty} \left(\frac{6\alpha}{\pi^2} \right)^l q_0^{2(1-l)} \quad (19)$$

In other words, the infinite series in Eq. (19) represents the correction to the TF result due to the introduction of exchange correlation. References 3 and 5 write Eqs. (16)–(18) with q replaced by Q , where Q differs from the TF result by terms in α and α^2 . This formal difference between q and Q emphasizes the problem of incompleteness inherent in the TFD treatment of these references. The use of Q in place of q overestimates the contraction of the screening radius from its TF value. For example, consider the case of pure exchange, $\alpha = \frac{2}{3}$. For silicon, q

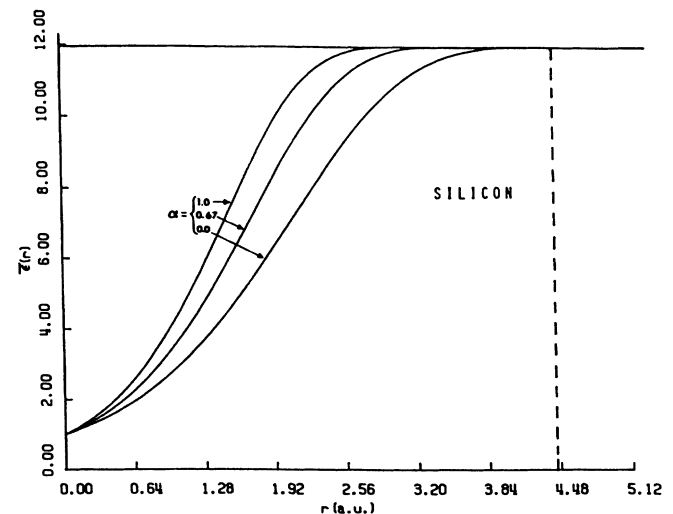


FIG. 1. Spatial dielectric functions for silicon in the linearized theory with the exchange-correlation strength as a parameter. The single-bond length (4.44) is denoted by the dashed line (all bond lengths in a.u.).

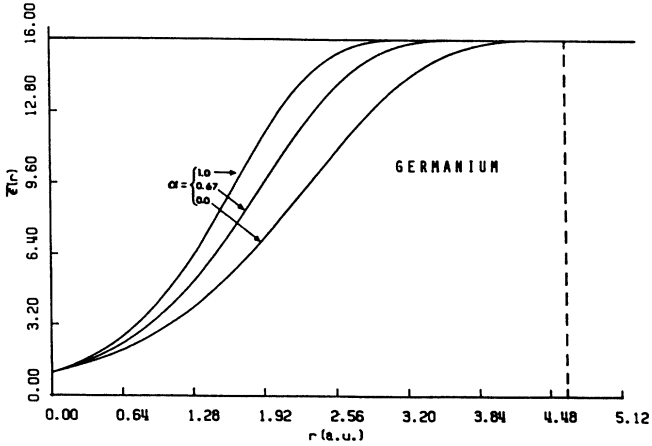


FIG. 2. Spatial dielectric functions for germanium in the linearized theory with the exchange-correlation strength as a parameter. The single-bond length (4.63) is denoted by the dashed line.

and Q have the values 1.35 and 1.47, respectively. The corresponding screening radii that follow from Eq. (18) are 3.5 and 3.22. The percent change in the screening radius from its TF value (4.28) is 18% and 25%, respectively. In this example, the use of q_0 , q , and Q leads to screening that is completed at about 96%, 79%, and 72% of the nearest-neighbor distance (4.44).

The spatial dielectric function given by Eqs. (17) and (18) is shown in Figs. 1–3 for silicon, germanium, and diamond, respectively. The behavior of $\bar{\epsilon}(r)$ is seen to be smooth and monotonic in r and approaches the macroscopic value $\epsilon(0)$ beyond the screening radius. As r approaches the origin, the curves go to unity, the value of the dielectric function in vacuum. As the exchange-correlation strength increases from its TF value of zero, the curves peak at lower values of r . Thus, with the inclusion of exchange correlation in the TF theory there is a more effective screening of the point impurity than

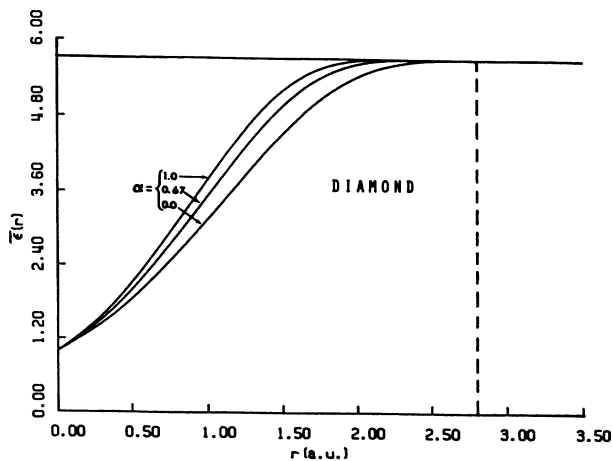


FIG. 3. Spatial dielectric functions for diamond in the linearized theory with the exchange-correlation strength as a parameter. The single-bond length (2.91) is denoted by the dashed line.

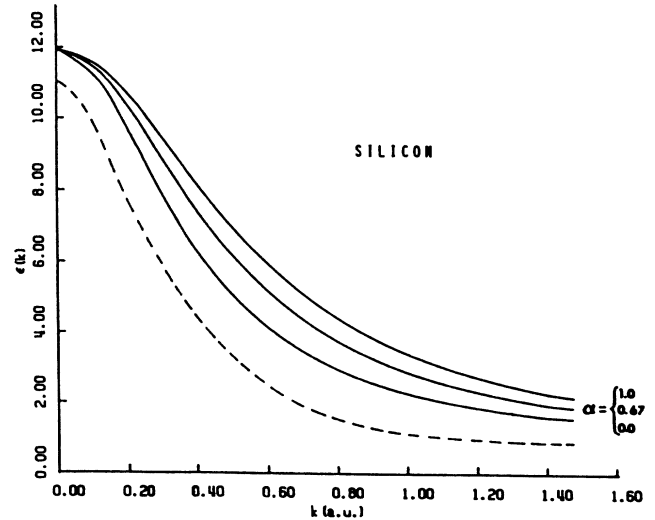


FIG. 4. Wave-vector-dependent dielectric functions for silicon in the linearized theory with the exchange-correlation strength as a parameter. The dashed line follows from the accurate band-structure calculations of Ref. 15.

without it. In other words, the screening electrons are drawn closer to the impurity as α increases. The same conclusion is reached in Refs. 3 and 5, even though the exchange-correlation part of E_F is absent.

The linear-response dielectric function in k space is defined as the ratio $v(k)/V(k)$, where $v(k)$ and $V(k)$ are the Fourier transforms of the unscreened and screened potentials, respectively. In the case of linearized TFD screening the dielectric function given in Eq. (17) yields the Fourier transform

$$\epsilon(k) = \frac{q^2 + k^2}{k^2 + [q^2 \sin(kR) + \epsilon(0)kR]} \quad (20)$$

The wave-vector-dependent dielectric functions predicted

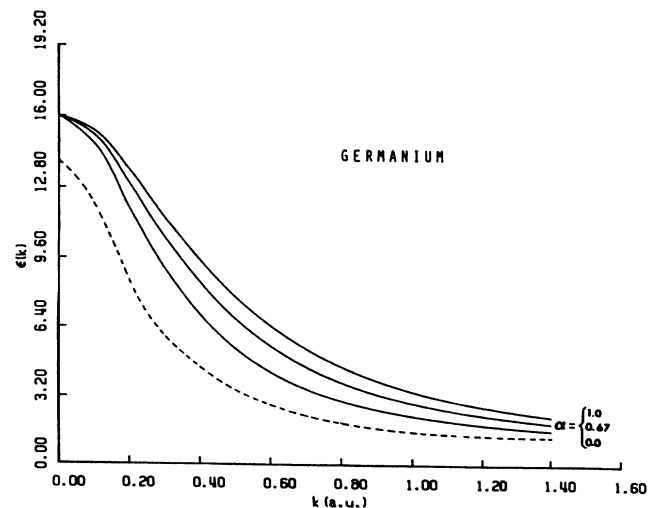


FIG. 5. Wave-vector-dependent dielectric functions for germanium in the linearized theory with the exchange-correlation strength as a parameter. The dashed line follows from the accurate band-structure calculations of Ref. 15.

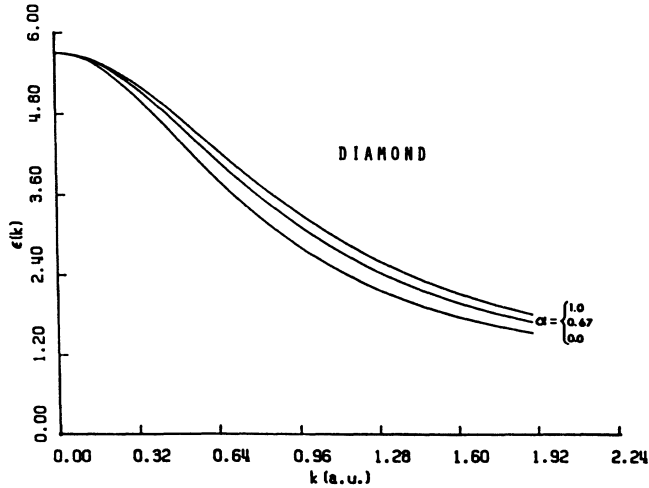


FIG. 6. Wave-vector-dependent dielectric functions for diamond in the linearized theory with the exchange-correlation strength as a parameter.

by Eq. (20) are shown in Figs. 4–6 for silicon, germanium, and diamond. The $\epsilon(k)$ curves are compared with the results of more sophisticated calculations of Walter and Cohen¹⁵ obtained on the basis of accurate band structure along the [100] direction in silicon and germanium. Figures 4 and 5 show that the wave-vector-dependent dielectric functions for silicon and germanium in the linear TF theory ($\alpha=0$) are in excellent agreement with results of Walter and Cohen, as noted by Resta.¹ These figures also show how the effects of exchange correlation tend to diminish this agreement.

III. VARIATIONAL CALCULATION OF SHALLOW-DONOR IONIZATION ENERGY

The shallow-donor ionization energy is calculated following the procedure outlined in Ref. 5. A single-conduction-band model semiconductor is treated in the effective-mass approximation. Thus, the one-donor-electron Hamiltonian consists of a kinetic-energy term with effective mass m^* , the screened impurity potential $V(r)$ [Eq. (16)], and a term $V_{xc}(r)$ embodying the exchange-correlation interaction of the impurity electron with the host valence electrons. To be consistent with the calculation of $V(r)$, the exchange-correlation potential must be formulated in the $X\alpha$ approximation. In that case,

$$V_{xc} = \begin{cases} -\frac{3}{2}\alpha \left[\frac{3n(r)}{\pi} \right]^{1/3}, & r \leq R \\ -\frac{3}{2}\alpha \left[\frac{3n}{\pi} \right]^{1/3}, & r \geq R \end{cases} \quad (21a)$$

$$(21b)$$

where $n(r)$ and n are given, respectively, by Eqs. (5) and (10). The quantities in large parentheses in Eqs. (21a) and (21b) are simply $k_F(r)$ and k_F , respectively. For $r \geq R$,

Eq. (21) coincides with Ref. 5 [Eq. (3.2)], since Eq. (2) is the basic relation between n and k_F . However, in the screening region, $r \leq R$, Ref. 5 [Eq. (3.2)] uses a form of $n(r)$ unlike Eq. (5) in that $V(R)$ [called $U(R)$ in Refs. 3 and 5] is shifted by the quantity $-B/Q^2$, where B is a fourth-degree polynomial in α with $E_F (=k_F^2/2)$ -dependent coefficients. This shift in $V(R)$ is a consequence of using an incomplete expression for the Fermi energy in the linearization procedure of Ref. 3.

As usual, the variational method provides an upper bound on the ionization energy, but it does suggest a trial wave function. In order to make comparisons with Ref. 5, a three-parameter unnormalized wave function $\psi(r)$, given by the sum of two exponentially decaying terms,

$$\psi(r) = e^{-\alpha_1 r} + b e^{-\alpha_2 r}, \quad (22)$$

will be used to calculate the expectation value of the Hamiltonian, \bar{H} . This quantity, divided by the normalization integral, is a function of the variational parameters α_1 , α_2 , and b . The host semiconductor is characterized by k_F , $\epsilon(0)$, and the effective mass m^* , while Z and α give flexibility for varying the ion charge state and the exchange-correlation effect. Specifically, electronic constants appropriate to silicon are used: $k_F=0.96$, $\epsilon(0)=11.94$, and $m^*=0.30$. The calculation of \bar{H} begins with a choice of Z . Then for a given value of α , the corresponding values of q and R are obtained from Eqs. (14) and (18), respectively. The Fermi energy follows from Eq. (1), for given k_F and α . All these quantities are fed into the expression for \bar{H} , which is then minimized. The only expectation integrals that could not be solved in closed form are those in the region $r \leq R$ of the exchange-correlation contribution to \bar{H} . These integrals were evaluated numerically using a 20-point Gaussian quadrature routine. A robust minimization procedure from the International Mathematical and Statistical Library was used in the numerical computation of \bar{H} . It involved a search for the minima of \bar{H} in three-parameter space and an evaluation of derivatives of \bar{H} with respect to the variational parameters. Optimum values of these parameters occur when all three derivatives are simultaneously as numerically close to zero as possible. The minimum value of \bar{H} is finally found by substituting these values back into the expression for \bar{H} . The whole procedure is repeated as α takes on various values in the range 0.0–1.0, including the TF or no exchange-correlation interaction ($\alpha=0.0$), the Kohn-Sham exchange potential ($\alpha=0.67$), and the Slater exchange potential ($\alpha=1.0$). As in Ref. 5, ionization energies are calculated with respect to the bottom of a conduction band of average exchange-correlation energy of a uniform electron gas of density n .

IV. RESULTS AND DISCUSSION

Numerical results of the minimization of \bar{H} with respect to the three variational parameters for four ion charges ($Z = +1, +2, +3, +4$) and for three values of the exchange-correlation strength α are presented in Table I. For comparison, the corresponding results given in Ref. 5 are also listed in parentheses. First, as expected,

TABLE I. Donor ionization energy for various charge states for $\alpha=0.0$ (no exchange potential), $\alpha=0.67$ (Kohn-Sham exchange potential), and $\alpha=1.00$ (Slater exchange potential). The energy is in hartrees. Schechter's values are in parentheses.

α	$Z = +1$	$Z = +2$	$Z = +3$	$Z = +4$
0.00	-0.001 092 (-0.001 092)	-0.005 343 (-0.005 346)	-0.028 179 (-0.026 52)	-0.172 394 (-0.173 0)
0.67	-0.001 097 (-0.001 097)	-0.005 531 (-0.005 278)	-0.033 879 (-0.023 07)	-0.203 912 (-0.143 7)
1.00	-0.001 096 (-0.001 103)	-0.005 465 (-0.005 402)	0.031 339 (-0.024 24)	-0.188 151 (-0.148 4)

it is seen that the TF ($\alpha=0.0$) values of the ionization energy are very close to those shown in parentheses. In the present case, the effect of exchange correlation is to make the energy levels deeper, regardless of the charge state. On the other hand, the results of Ref. 5 show that the effect of exchange correlation is to make the energy levels much shallower for $Z > +2$ and somewhat deeper for $Z < +2$.

The differences between the two sets of results are evinced further in Fig. 7 and Fig. 2 (Ref. 5), where the ratio of donor impurity ionization energy with exchange-correlation potential to the ionization energy without exchange correlation, $E(\alpha)/E(0)$, is plotted against α with ion charge as a parameter. From Fig. 7 it is concluded that when exchange correlation is included the energy levels get deeper as α starts increasing from zero. At values of α approaching unity, however, the energy levels tend to get shallower. This trend is mild for $Z = +1$ and $+2$, and quite strong for $Z = +3$ and $+4$. The energy levels lie deeper than the TF values over the entire range of α . A generally different behavior of the energy ratio is

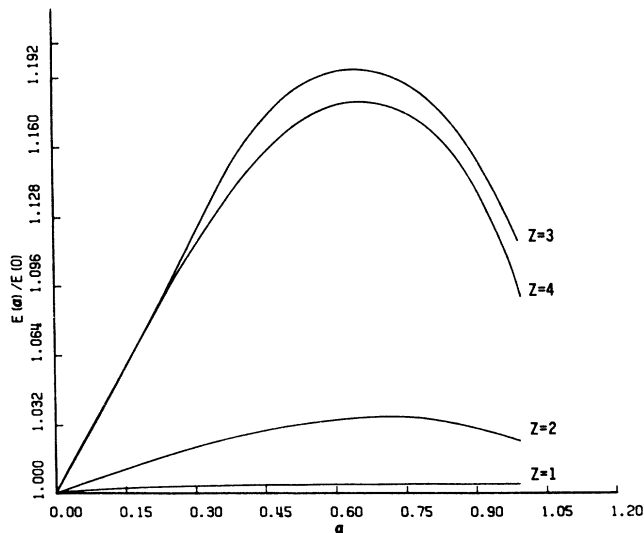


FIG. 7. Ratio of model donor impurity ionization energy with exchange-correlation strength α to the ionization energy without exchange, $E(\alpha)/E(0)$, as a function of α with impurity charge Z as a parameter.

seen in Fig. 2 (Ref. 5). There as α increases from zero, the energy levels get shallower, more so for $Z = +3$ and $+4$ than for $Z = +1$ and $+2$. In the former case, the trend reverses as α approaches unity, but the levels always remain above the TF values. In the latter case, the energy ratio eventually exceeds unity, implying that the energy levels then lie deeper than the TF values. As mentioned above, the present results for $V(r)$ and $n(r)$ in the linearized theory are different from the corresponding quantities in Refs. 3 and 5. These differences are manifest in the calculation of the shallow-donor ionization energy.

A shortcoming of the present treatment is undoubtedly its description of the exchange-correlation energy in the $X\alpha$ approximation. A more general approach rewrites the Euler equation [Eq. (9)] in the form

$$E_F = \frac{5}{3}c_k n^{2/3}(r) + V(r) - V(R) + \frac{\delta\epsilon_{xc}}{\delta n(r)}, \quad (23)$$

where the variation of the exchange-correlation energy density ϵ_{xc} is carried out in the local-density approximation. In the case where ϵ_{xc} is written as $(3\alpha/2)[n(r)]^{4/3}$, it is seen that the functional derivative generates the last term on the right-hand side of Eq. (9). A more accurate representation of ϵ_{xc} would, of course, be desirable, but it would lead to an analytically less convenient $n(r)$ -versus- $V(r)$ relationship than used here. Other approximate prescriptions for ϵ_{xc} have been given by Wigner,¹⁶ Hedin and Lundqvist,¹⁷ and Ceperley and Alder.¹⁸ The latter scheme has been parametrized by Perdew and Zunger¹⁹ and is considered to be the most accurate recipe for ϵ_{xc} . It remains for future numerical study to explore the use of these other forms of ϵ_{xc} in the TFD screening theory.

A more serious deficiency of the present theory is the fact that the kinetic-energy density is approximated by the local form proportional to the five-thirds power of the electron density. Since the main interest of this work concerns a consistent treatment of exchange correlation in the $X\alpha$ approximation within the TFD framework, corrections to the TF kinetic-energy functional are neglected entirely. A gradient expansion²⁰ of the kinetic energy gives the TF and TFD theories at zeroth order and one-ninth of the von Weizsäcker²¹ term as the second-order correction. The next contribution in the series is a fourth-order term given by Hodges.²² Approximations to the kinetic-energy functional based on a par-

tial summation of the gradient series have been considered.²³ Again, it remains for further investigation to add gradient corrections to the TF kinetic energy in the problem at hand. However, only limited success is expected because of questions concerning the general convergence properties of the gradient series. This extension and/or the use of a more accurate ϵ_{xc} will certainly lead beyond the convenient description of $V(r)$ offered by the single nonlinear Poisson equation given here. The TF and related theories are the precursors of modern density-functional theory²⁰ which allows for an exact treatment of the kinetic energy of a noninteracting electron gas. This approach involves the so-called Kohn-Sham²⁴ self-consistent equations, which include the Schrödinger equation and the associated single-particle wave functions. The application of this method is another way, of considerable interest, for finding $V(r)$. It represents the natural next step in the evolution of the solution of the impurity potential in a semiconductor. However, it lacks the attractiveness of the statistical method in which the electron density can be obtained directly from the potential.

In the present context, it is natural to think of extend-

ing the energy-level calculation to include the effects of nonlinearity. Nonlinear TFD screening of donor impurities in the $X\alpha$ approximation have been worked out numerically for various semiconductors in Ref. 12. Before proceeding with this application, it will be useful to fit these numerical results analytically for fixed values of Z and α . On the other hand, approximate analytical expressions for impurity potentials obtained from a variational principle equivalent of the nonlinear TFD screening equation may also be used for this purpose. From previous considerations of nonlinear TF (Ref. 2) and TFD (Ref. 4) screening, it is expected that $n(r)$ and thus $V(r)$ and $V_{xc}(r)$ will change substantially. As mentioned in Ref. 5, a significant alteration of the energy level is to be expected. This problem is presently under investigation.

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