

Weizsacker correction in the Thomas-Fermi and Thomas-Fermi-Dirac models of static dielectric screening in undoped semiconductors: Impurity donor ions in silicon and germanium

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Thomas-Fermi (TF- λ W) and Thomas-Fermi-Dirac (TFD- λ W) statistical models, including the Weizsacker gradient correction with variable coupling coefficient λ , have been applied to the problem of dielectric screening of an impurity donor ion in a homogeneous and isotropic semiconductor. Nonlinear differential Euler-Lagrange equations for the electron density are solved numerically and self-consistently with the impurity potential function under the screening charge constraint, giving microscopic response functions and screening radii with λ and ion-charge state as parameters. Illustrations of the numerical results are given for a monovalent donor point charge in silicon and germanium. It is evident that the TF- λ W and TFD- λ W screening radii are continuous, single-valued functions of λ with a minimum value in the range $0 \leq \lambda \leq 1$. Also, it is found that TF (TFD) and TF- $\frac{1}{9}$ W (TFD- $\frac{1}{9}$ W) spatial dielectric functions are in close agreement, the latter, however, having a smaller screening radius. The gradient correction reduces the nonlinear TF (TFD) screening radius by about 7.5% (9.8%) and 8.4% (12%), respectively, in silicon and germanium. Thus, the theoretical value, $\frac{1}{9}$, of λ leads to better results than the original value, 1, of Weizsacker which is associated with less effectively screened impurity potentials in both theories. The TF- $\frac{1}{9}$ W and TFD- $\frac{1}{9}$ W screening radii differ by about 20% for both semiconductors. It is expected that the nonlinear TFD- $\frac{1}{9}$ W screening functions will further improve the nonlinear TFD donor binding energies for silicon and germanium, which are already in quite good agreement with experiment. The TFD- λ W theory cannot be regarded as conclusive, since higher-order gradient corrections to the TF kinetic energy and gradient corrections to the Dirac exchange functional and the correlations functional, not to mention self-interaction effects, have not been taken into account here.

I. INTRODUCTION

The zero-temperature microscopic response of the valence electrons of an intrinsic semiconductor to a static substitutional point-charge impurity Z (in a.u.) has been investigated in terms of Thomas-Fermi¹ (TF: no exchange and correlation), Thomas-Fermi-Dirac² (TFD: pure exchange), and Thomas-Fermi-Dirac-Slater³ (TFDS: exchange and correlation in the $X\alpha$ approximation) statistical models. In each case minimization of the total ground-state energy functional with respect to the local electron density $n(r)$, subject to the constraint that the total number of electrons is constant, yields a Euler-Lagrange equation for $n(r)$ which must be solved self-consistently with the screened impurity $V(r)$ under the screening charge constraint. The displacement of the inhomogeneous electron density from the uniform, unperturbed background density n supplies the continuous source term in Poisson's equation for $V(r)$. This equation also contains a discrete source term associated with the point impurity. The Euler-Lagrange equation expresses the constancy of the electrochemical potential of the system and incorporates the boundary condition $n(R)=n$, where R is the finite radius of incomplete screening characteristic of the semiconductor. The quantity used to describe the dielectric response is the spatial dielectric function $\bar{\epsilon}(r)$, defined as the ratio of the bare

Coulomb potential, $-Z/r$, to the screened potential $V(r)$. Its properties include the boundary conditions $\bar{\epsilon}(0)=1$ and $\bar{\epsilon}(r)=\epsilon$, where ϵ is the macroscopic dielectric constant in the region of space $r \geq R$.

All three models may be derived together since the TF and TFD versions are straightforwardly obtained from the TFDS theory by simply setting the exchange-correlation parameter α equal to 0 (the no-exchange interaction) and $\frac{2}{3}$ (the Kohn-Sham exchange potential), respectively. The other frequently quoted value of α is 1, corresponding to the Slater exchange potential. The TFDS energy functional consists of the classical Coulomb potential energy of electron-electron and electron-nuclei interactions, plus kinetic and exchange-correlation energies based on locally planar electronic wave functions. The TF theory and its various modifications and improvements are the precursors of modern density-functional theory⁴ which provides a rigorous mathematical basis for showing that for ground states these models may be regarded as starting approximations to an exact many-electron theory. In density-functional theory all electronic properties of the ground state can in principle be determined by an exact constrained minimization of a unique energy functional of the local density. The Kohn-Sham version of this theory offers a practical set of equations for rigorous calculations.

Previous applications of the TF, TFD, and TFDS mod-

els to the problem of dielectric screening in semiconductors have ignored any consideration of gradient corrections to the kinetic and exchange-correlation energies. This paper is concerned, in particular, with the first gradient correction to the kinetic energy functional of the TF and TFD theories and its effect on the nonlinear dielectric response of a homogeneous and isotropic model semiconductor. The kinetic and exchange energy functional in these theories are obviously oversimplified by the local-density approximation which uses the corresponding uniform-electron-gas expressions through the local Fermi momentum. The Thomas-Fermi-Weizsacker (TF- λ W) and Thomas-Fermi-Dirac-Weizsacker (TFD- λ W) statistical models improve the TF and TFD kinetic energy functional by adding a gradient term with coupling coefficient λ . In the original work of Weizsacker,⁵ where λ is 1, this correction arises from allowing the electronic wave functions to be modified plane waves, thereby exhibiting effects of the inhomogeneity of the electron density. Formal gradient-expansion techniques⁶ have justified the Weizsacker term and provided higher-order⁷ gradient corrections to the kinetic energy. In these developments, however, the parameter λ is shown to be $\frac{1}{9}$ rather than 1. It is of interest to note in atomic and molecular applications that the TFD- λ W model overcomes some well-known difficulties associated with the TF and TFD descriptions, namely, the unphysical behavior of the electron density both near and asymptotically far from the nucleus, and the no-binding theorem which renders molecules impossible. Other values of λ besides 1 and $\frac{1}{9}$ are often used in these applications.⁸ The instability of negative ions and the lack of atomic shell structure are still serious shortcomings of the TFD- λ W theory.

One can think of adding correlation corrections to the TFD- λ W formalism. The Dirac-Slater local-density treatment of exchange in the $X\alpha$ approximation is a practical scheme for this purpose, as already shown by calculations carried out in papers II and III. The former uses a linearized version of the TFDS screening equation in an effective-mass variational calculation of shallow-donor impurity ionization energy, while the latter presents numerical and approximate analytical solutions of the complete TFDS screening equation with effects of nonlinearity and exchange correlation. Recent⁹ results show that donor binding energy is very sensitive to the form of dielectric screening. Binding energies obtained from numerical integration of Schrödinger's equation with nonlinear TFD screening of a monovalent donor impurity potential are in close agreement with experimental values for silicon and germanium. Better descriptions¹⁰ of the exchange-correlation energy and higher-order gradient corrections to the kinetic energy are desirable and available. In these cases, however, variational derivatives will lead to very complicated Euler-Lagrange equations for the electron density, not to mention that the sixth-order gradient correction to the TF kinetic energy for atoms diverges.¹¹ It remains for further work to investigate correlation effects by repeating the present calculations with the TFDS- λ W model, or some improvement thereof which incorporates correlation in a more sophisticated way. The Kohn-Sham equations are an alternate ap-

proach to the screening problem at hand. It would be of interest to calculate dielectric response functions with these equations and compare the results with those obtained through the present statistical methods. Another paper in this series is planned to report the results of this study.

The variational derivative of the TFD- λ W Euler-Lagrange equation is presented in Sec. II. The constant Lagrange multiplier used in this procedure to deal with the normalization condition on the electron density is identified with the electrochemical potential of the system. Both the screened impurity potential and the screening charge are expressed in terms of the electron density. The former relationship together with the Euler-Lagrange equation form the fundamental coupled system of equations. These are to be solved self-consistently under the screening charge constraint. The numerical method of solution described in Sec. III follows closely that used in TF- λ W and TFD- λ W theories of atoms. The nonlinear differential equation for the density function is solved by iteration of its linear form expressed in terms of finite differences. Linearized TF and TFD electron densities are used as initial density profiles and the screening radius is varied until convergence to a new density satisfies the polarization charge constraint. To ensure convergence, the iteration scheme is repeated with a linear superposition of the new and original densities as input until a consistent density and screening radius are found. Eventually, successive densities in this process satisfy the convergence criterion and yield the desired solution. Section IV presents numerical results obtained from the TF- λ W and TFD- λ W theories of dielectric screening in silicon and germanium. Screening radii for several values of λ and a corresponding subset of response functions, both parametrized by $Z = +1$, are displayed graphically. Considered as a continuous function of λ , it is seen that the screening radius, in both theories, is single-valued and possesses a minimum value in the interval $0 \leq \lambda \leq 1$. Section V gives a brief summary and some further remarks. 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 action (\hbar) are all set equal to unity. Because the theories under development here are isotropic, all space-dependent quantities are spherically symmetric functions of the magnitude r .

II. BASIC EQUATIONS OF THE TFD- λ W THEORY

A qualitative description of the TFD- λ W ground-state energy functional has been given in Sec. I. Its three basic components are kinetic, potential, and exchange energies. The kinetic energy density consists of a plane-wave electron contribution which is proportional to the five-thirds power of the electron density, and an inhomogeneity correction term which varies as the square of the gradient of the density. The exchange energy density in the plane-wave approximation is proportional to the four-thirds power of the density. Therefore, in the theory at hand, the total ground-state energy is expressed (in a.u.)

as

$$E = c_k \int n^{5/3}(r) d\tau + \lambda c_i \int \frac{[\nabla n(r)]^2}{n(r)} d\tau + \int n(r) V_N(r) d\tau + \frac{1}{2} \int n(r) V_e(r) d\tau - \frac{3}{2} \alpha c_e \int n^{4/3}(r) d\tau. \quad (1)$$

The exchange part of E has been expressed in the $X\alpha$ approximation. However, only the cases of no exchange ($\alpha=0$) and pure exchange ($\alpha=\frac{2}{3}$) are considered here since the focus is more on the effects of the gradient correction. The nuclear potential energy created by any nuclei is denoted by $V_N(r)$, while $V_e(r)$ is the potential energy due to the electron charge cloud. The mathematical expressions for these quantities are

$$V_N(r) = -\frac{Z}{r} - \int \frac{n d\tau'}{|\mathbf{r}-\mathbf{r}'|} \quad (2)$$

and

$$V_e(r) = \int \frac{n(r') d\tau'}{|\mathbf{r}-\mathbf{r}'|}. \quad (3)$$

The second term on the right-hand side of Eq. (2) originates from the positive-ion background prescribed by the usual jellium model. The total electrostatic potential energy $V(r)$ is identified as the sum $V_N(r) + V_e(r)$. The constant coefficients appearing in Eq. (1) are given by

$$c_k = \frac{3}{10} (3\pi^2)^{2/3}, \quad c_i = \frac{1}{8}, \quad c_e = \frac{3}{4} (3/\pi)^{1/3}. \quad (4)$$

The Euler-Lagrange equation follows from Eq. (1) by minimizing E with respect to variations in the density $n(r)$ while ensuring that the total number of electrons,

$$N = \int n(r) d\tau \quad (5)$$

remains fixed. This leads to the variational principle

$$\delta(E - [E_F + V(R)]N) = 0, \quad (6)$$

where E_F is the Fermi energy and where the electrochemical potential $E_F + V(R)$ plays the role of the Lagrange multiplier. The resulting master equation for the TFD- λ W model is

$$\frac{5}{3} c_k n^{2/3}(r) - 2\lambda c_i \left[\frac{\nabla^2 n(r)}{n(r)} - \frac{1}{2} \left(\frac{\nabla n(r)}{n(r)} \right)^2 \right] - \frac{4}{3} c_e n^{1/3}(r) + V(r) - E_F - V(R) = 0, \quad r \leq R. \quad (7)$$

For positive values of Z , there are two distinct regions of space around the impurity ion. The dispersive dielectric response of the semiconductor extends from the point probe located at the origin ($r=0$) to the screening distance R which is comparable to the nearest-neighbor distance. 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 macroscopic dielectric constant ϵ . For negative values of Z , the potential $V(r)$ becomes infinitely positive as r approaches the origin. This leads to the complication of a Coulomb hole, a physical region inside of which the electron density vanishes, leaving only the uniform background positive charge. TF and TFD

nonlinear screening equations for this problem have been solved and a rather remarkable donor acceptor asymmetry has been noted.^{1,2} For simplicity of presentation, the present paper deals exclusively with positive values of Z , especially the monovalent case. Another paper is planned for acceptor impurity ions in the TFD- λ W theory. Equations (2) and (3) show that $V(r)$ follows from electrostatic considerations. An equivalent way to accomplish this is to require that $n(r)$ and $V(r)$ are related by Poisson's equation

$$\nabla^2 V(r) = 4\pi[n - n(r)] + 4\pi Z \delta(r). \quad (8)$$

At this point, it is convenient to introduce the transformations $\rho(r) = rn^{1/2}(r)$ and $U(r) = rV(r)$. Then, a form of Eq. (7) suitable for numerical calculation is obtained. Namely,

$$4\lambda c_i \frac{d^2 \rho(r)}{dr^2} - \frac{5}{3} c_k r^{-4/3} \rho^{7/3}(r) + \frac{4}{3} c_e r^{-2/3} \rho^{5/3}(r) - \left[\frac{U(r)}{r} - E_F - \frac{U(R)}{R} \right] \rho(r) = 0, \quad r \leq R. \quad (9)$$

Equations (7) and (9) show that the inhomogeneity correction leads to a nonlinear differential equation for the electron density in terms of the potential. In the TF and TFD approximations, Eq. (9) reduces to an algebraic relationship between these quantities which conveniently combines with Poisson's equation to give the basic nonlinear differential equations for the screened potential in these theories. In these special cases, it follows directly from Eq. (9) that $\rho(r)$ vanishes as r tends to zero, while $\rho(r)$ is $R\sqrt{n}$ at $r=R$. These boundary conditions are maintained by Eq. (9) which is solved self-consistently with the potential function

$$U(r) = \frac{-Z}{\epsilon} + \frac{2\pi n}{3} (R-r)^2 (2R+r) - 4\pi \int_r^R \rho^2(r') dr' + 4\pi r \int_r^R \frac{\rho^2(r')}{r'} dr', \quad r \leq R \quad (10)$$

under the screening charge constraint

$$P(R) = 4\pi \int_0^R \rho^2(r) dr - \frac{4\pi}{3} nR^3 - Z \left[1 - \frac{1}{\epsilon} \right] = 0. \quad (11)$$

Equation (10) embodies all the properties expected of $U(r)$. Twice differentiated with respect to r , it reproduces Poisson's equation for $U(r)$. In the limit as r tends to zero, it shows that $U(r)$ approaches its unscreened value, $-Z$. Continuity of both the electric potential and the electric field, at the screening radius R , are guaranteed by Eq. (10). Equations (9) and (10) are the basic equations of the TF- λ W and TFD- λ W models with $c_e=0$ in the former.

The complete analogy between TF screening in a metal and a semiconductor and the TF theory of atoms and positive ions, respectively, has been noted by Resta.¹ TF metals and atoms are alike in that the screening charge extends over the entire crystal and all space, respectively. On the other hand, TF semiconductors and positive ions have in common the existence of a finite screening radius

and a finite ionic radius, respectively. It goes without saying that this analogy is also enjoyed by the TFD, TFDS, TF- λ W, TFD- λ W, and TFDS- λ W extensions of the Thomas-Fermi theory. Application of these various models to the problem of impurity screening in metals also is a subject of relevant interest. In this regard, it has been shown¹² that the linearized TF approximation, the nonlinear TF theory, and the nonlinear TFD model lead progressively to more effective screening of a positive impurity. Since these investigations also are without consideration of correlation effects and gradient corrections, it may be useful to study this problem within the context of the TFDS- λ W description of screening.

III. NUMERICAL METHOD OF SOLUTION OF THE NONLINEAR TFD- λ W EQUATIONS

There are basically two main approaches to the numerical solution of the nonlinear TFD- λ W equations, namely, the finite-difference method¹³ and the spline-representation method.¹⁴ This paper works with the first scheme and follows the procedure used by several authors.¹³ A very effective way for solving Eqs. (9) and (10) deals with the linearization of Eq. (9). This is done by letting $\rho(r) = \rho_0(r) + \Delta\rho(r)$ and neglecting higher-order terms in the small quantity $\Delta\rho(r)$. Under these conditions, formal expansion of Eq. (9) yields

$$4\lambda c_i \frac{d^2\rho(r)}{dr^2} - \left[\frac{35}{9} c_k r^{-4/3} \rho_0^{4/3}(r) - \frac{20}{9} c_e r^{-2/3} \rho_0^{2/3}(r) + \frac{U(r)}{r} - \frac{U(R)}{R} - E_F \right] \rho(r) = -\frac{20}{9} c_k r^{-4/3} \rho_0^{7/3}(r) + \frac{8}{9} c_e r^{-2/3} \rho_0^{5/3}(r), \quad r \leq R \quad (12)$$

which is then replaced by a set of second-order difference equations and solved by iteration until convergence is reached. The procedure is as follows. (1) Make an initial guess for the screening radius R^0 and set up a uniformly spaced radial grid r_i ($i = 1, 2, \dots, M$) with the assignments $r_1 = 0$ and $r_M = R^0$. Discretize the density function $\{\rho_i\}$ on this grid with boundary conditions $\rho_1 = 0$ and $\rho_M = R^0 n^{1/2}$. (2) Use linearize TF and TFD results to ob-

tain a starting form $\rho_0^0(r)$ for the density profile $\rho_0(r)$. The former is given by

$$\rho_{0i}^0(r) = r_i \left[(2^{3/2}/3\pi^2) \left[E_F - \frac{Z}{R^0 \epsilon} + \frac{Z}{r_i \bar{\epsilon}(r_i)} \right]^{3/2} \right]^{1/2}, \quad r_i \leq R^0 \quad (13)$$

where the spatial dielectric function in Eq. (13) has the form

$$\bar{\epsilon}(r_i) = \epsilon q R^0 / \{ \sinh[q(R^0 - r_i)] + q r_i \}. \quad (14)$$

The input parameters are the point-ion charge Z , the Weizsacker coupling coefficient λ , the static dielectric constant ϵ , and the valence Fermi momentum k_F . Characteristic quantities for silicon and germanium are given in Table I. (3) Compute the corresponding potential function $\{U_i^0(r)\}$ of Eq. (10). (4) With R^0 and $\{U_i^0\}$ solve Eq. (9) by iterating Eq. (12), each iteration requiring the solution of a tridiagonal system of equations, until convergence to a new density $\{\rho_{0i}^1\}$ is achieved. (5) Use $\{\rho_{0i}^1\}$ to check the charge constraint, Eq. (11). If it is not satisfied, the whole process is repeated with a new value of the screening radius until the density represented by some $\{\rho_{0i}^m\}$ satisfies Eq. (11). To assure convergence, the new $\{\rho_{0i}^m\}$ are mixed equally with the original $\{\rho_{0i}^0\}$ to form the next guess $\{\rho_{0i}^1\}$ as input to step (3). The iteration scheme is repeated until a consistent $\{\rho_{0i}^m\}$ and screening radius are found. The entire procedure continues until consecutive solutions converge to within an accuracy of $|\Delta\rho_i/\rho_i| \leq 10^{-4}$, giving the desired result.

The following features of the numerical method are noted. (1) The initial R was selected such that $P(R) > 0$. The screening radius was then decreased in increments of 0.01 until $P(R) < 0$, thereby establishing a reasonably small R interval within which $P(R)$ vanishes. At this stage, a bisection routine was used to continue the solution process. (2) The screening radius and the potential function are held fixed during the iteration under step (4). (3) The boundary conditions on the density function are maintained throughout the calculation. (4) The calculations reported here employ $M = 1000$. The grid spacing is a function of R and typically converges between 0.002 and 0.004.

TABLE I. Listing of physical parameters and characteristic quantities concerning the linearized TF and TFD models of dielectric screening in silicon and germanium.

	Silicon	Germanium
Nearest-neighbor distance (a.u.)	4.44	4.63
Static dielectric constant ϵ	11.94	16.0
Valence Fermi momentum k_F (a.u.)	0.96	0.98
Uniform valence electron gas density $n = k_F^3/3\pi^2$	0.0296	0.0318
$E_F^{\text{TF}} = k_F^2/2$	0.461	0.480
$E_F^{\text{TFD}} = E_F^{\text{TF}} - k_F/\pi$	0.155	0.168
$q_{\text{TF}} = (4k_F/\pi)^{1/2}$	1.106	1.117
$q_{\text{TFD}} = q_{\text{TF}} [k_F/(k_F - 1/\pi)]^{1/2}$	1.352	1.359
TF screening radius (a.u.)	4.280	4.540
TFD screening radius (a.u.)	3.500	3.740

IV. NUMERICAL RESULTS AND DISCUSSION

In a previous paper, I, the nonlinear TFD screening equation for the electron-gas-model semiconductor has been solved numerically, giving both spatial dielectric functions and screening radii with an ion charge as the parameter. The results for impurity donor ions show a reduction in the TF screening radii, meaning that attractive potentials are more effectively screened in the TFD theory. For acceptor ions, TF screening radii and Coulomb-hole radii are reduced and increased, respectively, showing that repulsive potentials are enhanced in the TFD theory. A more recent paper, III, gives the numerical solution of the nonlinear TFDS screening equation for donor ions and includes a variational principle equivalent which leads to approximate analytical expressions for the dielectric functions in close agreement with the exact results. It is found that a continuous increase in the exchange-correlation parameter from 0 to 1 correspondingly reduces the screening radii and attractive potentials set up around donor ion-charges.¹⁵ Linearized versions of TF, TFD, and TFDS theories yield closed analytical expressions for both wave-vector and spatial dielectric functions. In this regime, these Z -independent quantities already make manifest the screening trends described above.

The nonlinear TFDS- λ W theory provides an opportunity for investigating the behavior of R and $\bar{\epsilon}(r)$ as functions of the Weizsacker coupling coefficient and the exchange-correlation strength, for various values of the ion charge. For present purposes, the discussion is restricted to the TF- λ W and TFD- λ W models. The numerical method described in Sec. III, for solving these cases, has been applied to the screening of a monovalent donor ion in silicon and germanium. Screening radii and dielectric functions have been calculated for nine values of λ ($0, \frac{1}{9}, \frac{1}{4}, \frac{3}{8}, \frac{1}{2}, \frac{5}{8}, \frac{3}{4}, \frac{7}{8}, 1$). Figure 1 shows a comparison between TF ($\alpha=0; \lambda=0$) and TF- λ W ($\alpha=0; \lambda=\frac{1}{9}, 1$) screening functions for silicon [Fig. 1(a)] and germanium [Fig. 1(b)], parametrized by $Z=+1$. In each figure, the vertical (dotted-dashed) line defines the single-bond length characteristic of the semiconductor. The dotted and solid curves represent TF and TF- λ W results, respectively. In the latter case, the Weizsacker ($\lambda=1$) screening function has the smaller values over most of its length. Although the screening radius associated with this function is the smallest of the three radii in each of these figures, it is seen that the impurity potential is less effectively screened for $\lambda=1$. The close agreement between the TF and TF- $\frac{1}{9}$ W screening functions is especially noteworthy. Calculations⁹ of donor binding energies in these semiconductors show that better results are obtained as the impurity potential is more effectively screened in the following order: linear TF, nonlinear TF, linear TFD, and nonlinear TFD. It follows that the value of λ which is justified by formal gradient expansions of the kinetic energy is the appropriate one to use here. In that case, the main consequence of the gradient term is to reduce the screening radius from its TF value (4.060 for silicon and 4.330 for germanium) by about 7.5% and

8.4% in silicon (3.757) and germanium (3.965), respectively.

Figure 2 gives a comparison between nonlinear TFD ($\alpha=\frac{2}{3}; \lambda=0$) and nonlinear TFD- λ W ($\alpha=\frac{2}{3}; \lambda=\frac{1}{9}, 1$) screening functions for silicon [Fig. 2(a)] and germanium [Fig. 2(b)], parametrized by $Z=+1$. The dotted and solid curves represent TFD and TFD- λ W results, respectively. In the latter case, the Weizsacker ($\lambda=1$) dielectric function has the smaller values between the limits 1 and ϵ . Also, it has the largest screening radius of the three radii in each of these figures, and tends to enhance the impurity potential over its entire length. The close correspondence between the TFD and TFD- $\frac{1}{9}$ W dielectric function, again, shows that the natural choice of λ is $\frac{1}{9}$. On the basis of results obtained in Ref. 9, it is concluded that impurity potentials derived from these gradient-corrected functions will lead to preferred binding energies in these semiconductors. The gradient term reduces the TFD screening radius (3.340 for silicon and 3.600 for germanium) by about 9.8% and 12% in silicon (3.014) and germanium (3.158), respectively.

Screening radii for a monovalent donor ion and nine values of λ , in the range of $0 \leq \lambda \leq 1$, are displayed graph-

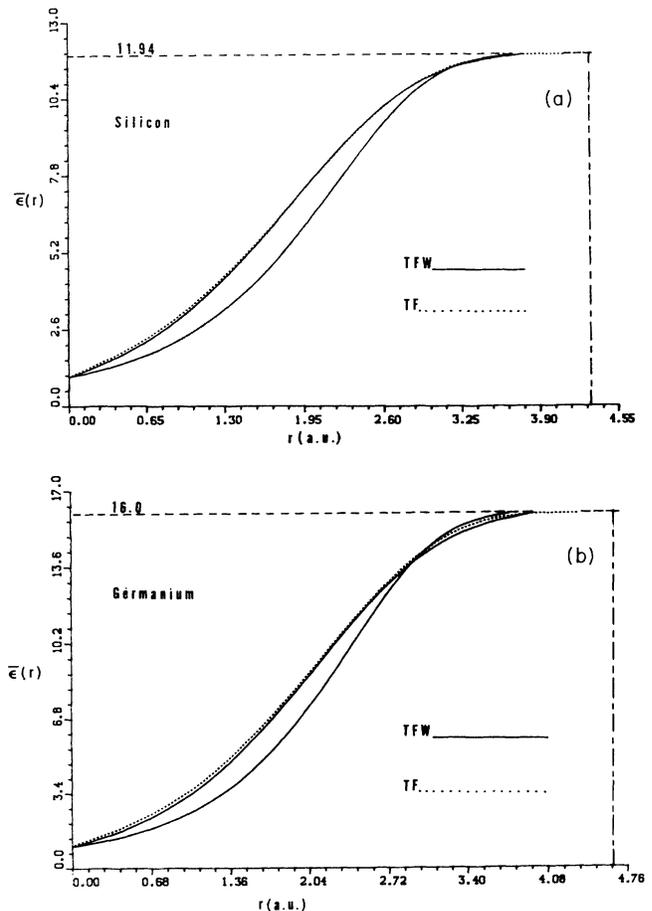


FIG. 1. Exact spatial dielectric functions for silicon (a) and germanium (b) for the monovalent donor ion-charge state in the nonlinear regimes of TF and TF- λ W screening theory.

ically in Fig. 3 for silicon [Fig. 3(a)] and germanium [Fig. 3(b)]. It is evinced from the TF- λ W and TFD- λ W data in these figures that the screening radius begins with its largest value at $\lambda=0$, decreases with increasing λ until a minimum value is reached, and then increases beyond that point. Thus, in some instances two different values of λ lead to the same screening radius. The TF ($\lambda=0$), Weizsacker (TF-1W), and theoretically preferred (TF- $\frac{1}{9}$ W) screening radii identified in Fig. 1, and corresponding TFD- λ W quantities in Fig. 2, occur as subsets of the numerical data in Fig. 3. It is clear that TFD- λ W screening radii are smaller than their TF- λ W counterparts for all values of λ in the range under consideration. In particular, a comparison between TF- $\frac{1}{9}$ W and TFD- $\frac{1}{9}$ W screening radii shows a difference of about 20% for both semiconductors. Dielectric functions for values of λ other than 0, $\frac{1}{9}$, and 1 are not illustrated here for simplicity of presentation.

It is straightforward to apply the numerical method of Sec. II to the screening of divalent, trivalent, and tetravalent donor impurity ions in silicon and germanium. Without going through a repetitious discussion of the results, it is noted that TF- λ W and TFD- λ W screening radii, parametrized by these donor ion-charge states, are

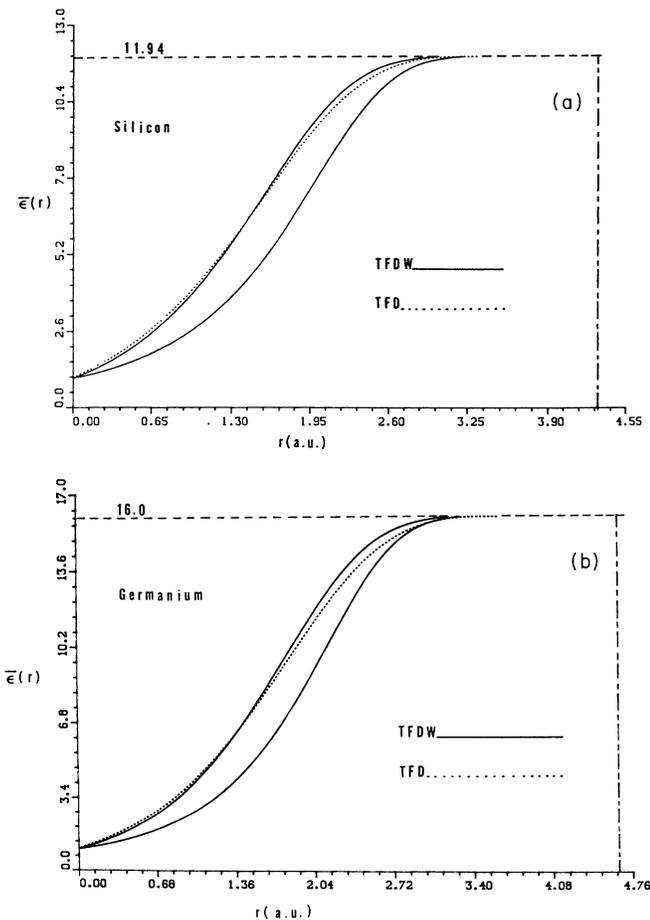


FIG. 2. Exact spatial dielectric functions for silicon (a) and germanium (b) for the monovalent donor ion-charge state in the nonlinear regimes of TFD and TFD- λ W screening theory.

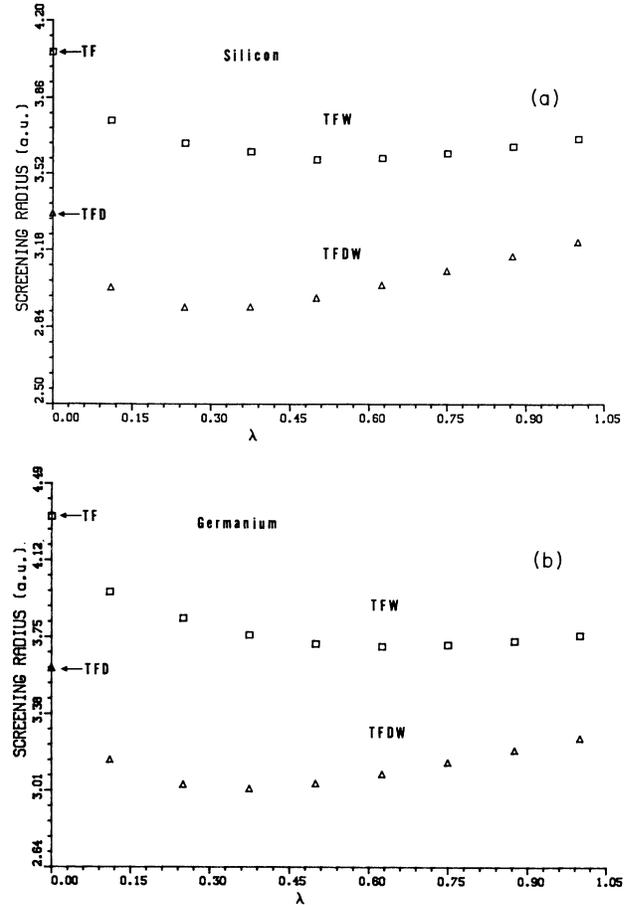


FIG. 3. Screening radii in silicon (a) and germanium (b) vs nine values of the gradient coupling coefficient (λ) in the nonlinear regimes of TF- λ W and TFD- λ W screening theory for a monovalent donor ion.

single-valued functions of λ , in the range $0 \leq \lambda \leq 1$, which generally behave like the monovalent curves. In both theories, the screening radius decreases as Z increases, for a given value of λ . For example, the TF- $\frac{1}{9}$ W screening radius in silicon and germanium, for $Z = +1$, is about 5% larger than its value for $Z = +4$. Similarly, the TFD- $\frac{1}{9}$ W screening radii in silicon and germanium, for $Z = +1$, are about 13% and 11% larger, respectively, than their values for $Z = +4$. Full numerical results concerning these other charge states will be reported elsewhere. Also, semiconductors such as carbon, gallium arsenide, gallium phosphide, and $\text{Ga}_{1-x}\text{Al}_x\text{As}$ are readily included in the investigation initiated here. Linear and nonlinear TF and TFD models of dielectric screening in these semiconductors already have been developed in the literature for various donor and acceptor ions. Numerical work dealing with these semiconductors is in progress.

V. SUMMARY AND FURTHER REMARKS

The TF- λ W and TFD- λ W descriptions of impurity screening in semiconductors (and metals) represents a generalization of previous applications of TF and TFD

methods to these problems in that an attempt is made in the former to include effects of the inhomogeneous electron gas. Mathematically, this modification appears through the presence of an additional term in the TF and TFD Euler-Lagrange equations for the electron density which converts them from nonlinear algebraic to nonlinear differential equations to be solved self-consistently with the potential function, subject to charge constraint and proper boundary conditions. The latter equations are linearized and expressed in finite-difference form for numerical solution by successive iteration. Linearized TF and TFD electron density profiles, with known analytical forms, serve as input data for this solution process. Results for silicon and germanium concerning a monovalent donor impurity show that nonlinear TF- $\frac{1}{9}W$ and TFD- $\frac{1}{9}W$ response functions are in close agreement with their TF and TFD counterparts, except that the former have smaller screening radii than the latter. This is a satisfactory result for at least two reasons: (1) the natural value of λ is $\frac{1}{9}$ and (2) nonlinear TFD dielectric functions lead to binding energies for silicon and germanium that are quite close to experimental values. The reduction in screening radii accompanying the nonlinear TFD- $\frac{1}{9}W$ response functions is expected to further improve this already good agreement.

The TFD- λW theory cannot be regarded as a complete description of screening in semiconductors and metals, no more than it can be considered as a rigorous approach

to atomic and molecular structure. The inhomogeneity correction included in this work is concerned solely with the second-order contribution to the TF kinetic energy. Aside from higher-order terms in the gradient expansion of this energy, also there are gradient corrections¹⁶ to the Dirac exchange energy, not to mention the correlation energy. It is of obvious interest to introduce the standard second-order exchange inhomogeneity correction into the total-energy functional and study its effect on the present numerical results. This problem is currently under investigation. Another source of difficulty with the approximate energy functional of Eq. (1) is that both the electron-electron interaction and the exchange-correlation energy contain spurious self-interaction effects. A proposed solution of this problem gives reasonable results in atomic calculations,¹⁷ but difficulties remain, especially the elimination of self-interaction effects in extended systems.¹⁸

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- ¹R. Resta, Phys. Rev. B **16**, 2717 (1977); F. Cornolti and R. Resta, *ibid.* **17**, 3239 (1978).
- ²P. Csavinsky, Phys. Rev. B **28**, 6076 (1983); L. M. Scarfone, *ibid.* **29**, 3259 (1984), henceforth referred to as I; **32**, 2653 (1985); D. Chandramohan and S. Balasubramanian, *ibid.* **33**, 8782 (1986).
- ³A. Enver and L. M. Scarfone, Phys. Rev. B **41**, 10642 (1990); L. M. Scarfone and A. Enver, *ibid.* **43**, 2272 (1991); henceforth referred to as II and III, respectively.
- ⁴See, for example, J. Callaway and N. H. March, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1984), Vol. 38, p. 135; *Theory of the Inhomogeneous Electron Gas*, edited by S. Lundqvist and N. H. March (Plenum, New York, 1983).
- ⁵C. F. Weizsacker, Z. Phys. **96**, 431 (1935).
- ⁶See discussion and references in R. G. Parr and W. Yang, *Density-Functional Theory of Atoms and Molecules* (Oxford, New York, 1989); E. H. Lieb, Rev. Mod. Phys. **53**, 603 (1981).
- ⁷C. H. Hodges, Can. J. Phys. **51**, 1428 (1973); D. R. Murphy, Phys. Rev. A **24**, 1682 (1981).
- ⁸K. Yonei and Y. Tomishima, J. Phys. Soc. Jpn. **20**, 1051 (1965); Y. Tomishima and K. Yonei, *ibid.* **21**, 142 (1966); E. H. Lieb, Ref. 6; W. Jones and W. H. Young, J. Phys. C **4**, 1322 (1971); M. Brack, in *Density Functional Methods in Physics*, edited by R. M. Dreizler and J. da Providencia (Plenum, New York, 1985), p. 331.
- ⁹Y. P. Varshni and S. M. Khanna, Phys. Rev. B **43**, 9279 (1991).
- ¹⁰E. P. Wigner, Phys. Rev. **46**, 1002 (1934); L. Hedin and B. I.

- Lundqvist, J. Phys. C **4**, 2064 (1971); D. M. Ceperly and B. J. Adler, Phys. Rev. Lett. **45**, 566 (1980).
- ¹¹D. R. Murphy, Ref. 7; Y. Tal and R. F. W. Bader, Int. J. Quantum Chem. Symp. **12**, 153 (1978).
- ¹²N. F. Mott, Proc. Cambridge Philos. Soc. **32**, 281 (1936); J. Friedel, Adv. Phys. **3**, 44 (1954); L. C. R. Alfred and N. H. March, Philos. Mag. **46**, 759 (1955); H. Fujiwara, J. Phys. Soc. Jpn. **11**, 376 (1956); N. H. March, Adv. Phys. **6**, 1 (1957); A. Sjölander and M. J. Stott, Phys. Rev. B **5**, 2109 (1972); C. O. Almbladth, V. von Barth, Z. D. Popovii, and M. J. Stott, *ibid.* **14**, 2250 (1976).
- ¹³K. Yonei and Y. Tomishima, Ref. 8; Y. Tomishima and K. Yonei, Ref. 8; W. Yang, Phys. Rev. A **34**, 4575 (1986); A. M. Abrahams and S. L. Shapiro, *ibid.* **42**, 2530 (1990).
- ¹⁴A. Stich, E. K. U. Gross, P. Malzacker, and R. M. Dreizler, Z. Phys. A **309**, 5 (1982).
- ¹⁵TFDS screening theory of acceptor ions is covered by A. Enver, Ph.D. thesis, University of Vermont, 1988. Also, see D. Chandramohan and S. Balasubramanian, Z. Phys. B **79**, 181 (1990).
- ¹⁶L. J. Sham, in *Computational Methods in Band Theory*, edited by P. J. Marcus, J. F. Janak, and A. D. Williams (Plenum, New York, 1971); E. K. U. Gross and R. M. Dreizler, Z. Phys. A **302**, 103 (1981).
- ¹⁷J. P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).
- ¹⁸See discussion and references in J. Callaway and N. H. March, *Solid State Physics* (Ref. 4), p. 182.