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Thomas-Fermi-Dirac dielectric function for GaAs and GaP

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The nonlinear Thomas-Fermi-Dirac equation is solved numerically for the positive and negative point charges in gallium arsenide and gallium phosphide. Results are obtained for screening radii, Coulomb hole radii, and spatial dielectric functions which are compared with those obtained by solving the nonlinear Thomas-Fermi equation. The inconsistency in the definition of the Coulomb hole radius, observed earlier, has been taken care of. The wave-vector-dependent dielectric function and the spatial dielectric function are also obtained for the linear case and its range of validity given.

I. INTRODUCTION

Resta[1] has developed a nonlinear Thomas-Fermi (TF) theory of the screening of point impurity charges in semiconductors at zero temperature. Cornolti and Resta[2] have numerically solved Resta's nonlinear equation and have presented graphically results for $\epsilon(r)$, the spatial dielectric function, for point charges $Z=\pm 1, \pm 4$ (in atomic units) in diamond, silicon, and germanium. Similar calculations were made by Chandramohan and Balasubramanian[3] for GaAs and by Singh and Balasubramanian for GaP (Ref. 4) and other semiconductors.[5] The TF model dielectric functions obtained by Resta are in good agreement with the accurate pseudopotential random-phase-approximation calculations of Walter and Cohen[6] made in wave-vector space. Csavinszky and Brownstein[7] and Csavinszky and Elabsy[8] have calculated the dielectric function by a variational method in the TF theory. Recently Scarfone[9,10] has formulated a nonlinear Thomas-Fermi-Dirac (TFD) theory of dielectric screening in undoped semiconductors at zero temperature. In his formulation, Scarfone has introduced corrections to the TF theory of dielectric screening by taking into account the effects of exchange. Scarfone has solved the nonlinear TFD equation numerically for $Z=\pm 1, \pm 2, \pm 3, \pm 4$ in diamond, Si, and Ge.

There was some discrepancy in Ref. 9 in the case of negative point-charge impurities which was rectified by Scarfone in the subsequent work.[10] An inconsistency in the definition of the Coulomb-hole radius for the negative point charges in Refs. 9 and 10 has been recently pointed out by the present authors.[11] It has been noted that the above inconsistency has no noticeable consequence on the dielectric function for diamond, while for Si and Ge, there has been some noticeable change.

It would be of interest to do calculations on the dielectric functions for compound semiconductors GaAs and GaP using the TFD theory. The screened impurity potentials in these materials are useful in calculating the impurity states as well as ionized-impurity-limited mobilities of the carriers.[12] Positive charges would correspond to donors and negative charges to acceptors. In the present work, the nonlinear TFD equation is solved numerically for $Z=\pm 1, \pm 2, \pm 3, \pm 4$ in GaAs and GaP. Results are obtained for the screening radii, Coulomb-hole radii, and spatial dielectric functions. These are compared with the results based on the nonlinear TF equation without exchange. The wave-vector-dependent dielectric function $\epsilon(k)$ and the spatial dielectric function are also obtained for the linearized case. Atomic units are used throughout the paper, so that e, $\hbar$, and m_0 equal 1. Section II contains a brief outline of the theory and Sec. III has the results and discussions.

II. TFD SCREENING EQUATION

We consider the valence electrons in a semiconductor as a Fermi gas with electron density n. When a point charge is introduced, the redistributed charge density $n(r)$ is related to the screened potential $V(r)$ by Poisson's equation,

$$-\nabla^2 V(r) = 4\pi[n(r) - n] \ . \tag{1}$$

In the TFD theory we have[9]

$$n = \frac{2^{3/2}}{3\pi^2}[\gamma + (\gamma^2 + E_F)^{1/2}]^3 \ . \tag{2}$$

For the positive point charge $+Z$,

TABLE I. Listing of physical parameters and characteristic quantities entering in the linearized TF and TFD models of dielectric screening for GaAs and GaP.

	GaAs	GaP
Nearest-neighbor distance a (a.u.)	4.62	4.46
Static dielectric constant K_0	12.56	11.02
Valence Fermi momentum k_F (a.u.)	0.92	0.95
$(E_F)_{\rm TF} = k_F^2/2$ (a.u.)	0.42	0.45
E_F(a.u.)$= k_F^2/2 - k_F/\pi$	0.13	0.15
Screening radius R (a.u.)	3.57	3.43

TABLE II. Listing of various measures of the range of validity of the linearized TF and TFD screening equations for GaAs and GaP when $Z=1$ and $Z=2$. TF values are in parentheses.

	GaAs		GaP	
	$Z=1$	$Z=2$	$Z=1$	$Z=2$
r_0 (a.u.)	1.16 (0.90)	1.49 (1.24)	1.11 (0.86)	1.44 (1.19)
r_0/a	0.25 (0.19)	0.32 (0.27)	0.25 (0.19)	0.32 (0.27)
r_0/R	0.33 (0.20)	0.42 (0.28)	0.32 (0.20)	0.42 (0.28)
$\epsilon(r_0)$	4.24 (2.53)	5.96 (3.51)	3.94 (2.47)	5.52 (3.39)
$[\epsilon(r_0)/K_0]$ (100%)	33.76 (20.1)	47.45 (27.90)	35.75 (22.41)	50.09 (30.76)

$$n(r)=\begin{cases}\dfrac{2^{3/2}}{3\pi^2}\{\gamma+[(-\gamma)^2+E_F+V(R)-V(r)]^{1/2}\}^3, & r\le R\\ n, & r>R\end{cases}\tag{3}$$

and for the negative point charge $-Z$,

$$n(r)=\begin{cases}0, & 0<r\le R_C\\ \dfrac{2^{3/2}}{3\pi^2}\{\gamma+[(-\gamma)^2+E_F+V(R)-V(r)]^{1/2}\}^3, & R_c<r\le R\\ n, & r>R\ .\end{cases}\tag{4}$$

In Eqs. (3) and (4), γ is a constant equal to $1/2^{1/2}\pi$, R is the screening radius, E_F is the valence Fermi energy including the exchange correction, and $V(R)=\mp Z/K_0R$, K_0 being the static dielectric constant of the semiconductor. The Coulomb-hole radius R_c in Eq. (4) is defined by[11]

$$V(R_C)=E_F+V(R)\ .\tag{5}$$

Equation (1) is in general nonlinear and can be solved numerically with appropriate boundary conditions. Ana-

TABLE III. Listing of screening radii and Coulomb-hole radii for nonlinear TFD screening equation when $Z=\pm1$, ±2, ±3, and ±4. TF values are in parentheses, and $Z=0$ corresponds to the linear results of Table I.

Z	GaAs	GaP
	Screening radius R (a.u.)	
4	3.19 (3.86)	3.04 (3.66)
3	3.25 (3.95)	3.10 (3.74)
2	3.32 (4.05)	3.18 (3.85)
1	3.42 (4.19)	3.27 (3.98)
0	3.57 (4.44)	3.43 (4.20)
-1	4.00 (4.81)	3.84 (4.57)
-2	4.31 (5.08)	4.13 (4.83)
-3	4.56 (5.30)	4.37 (5.04)
-4	4.77 (5.49)	4.57 (5.22)
	Coulomb-hole radius R_C (a.u.)	
-1	1.53 (1.03)	1.45 (0.98)
-2	2.07 (1.52)	1.97 (1.46)
-3	2.45 (1.88)	2.34 (1.80)
-4	2.76 (2.16)	2.63 (2.08)

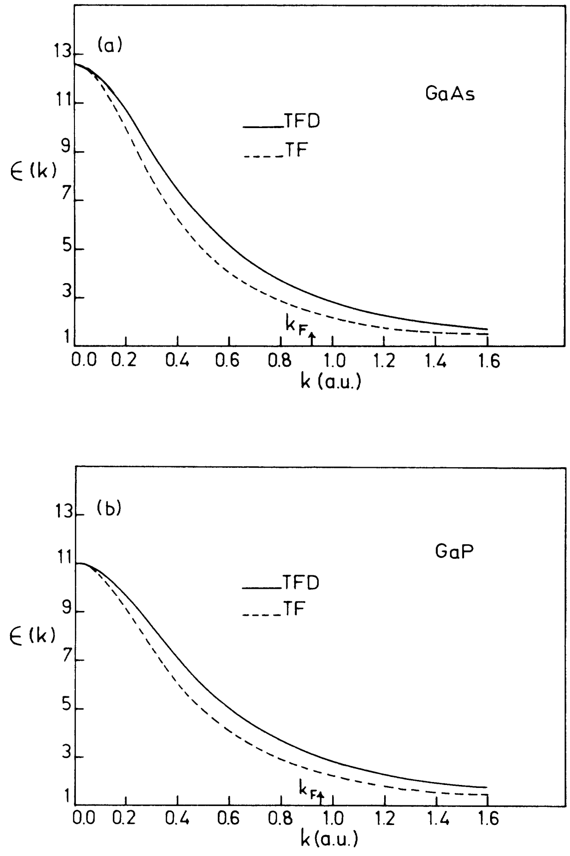

FIG. 1. TF and TFD wave-vector-dependent dielectric functions in the linearized model.

lytic solution may be obtained for the linearized equation; the linearization involves a binomial expansion in which the square of $[V(R)-V(r)]/(\gamma^2+E_F)$ is neglected in comparison with unity. The linearization is valid only when

$$\left|\frac{V(R)-V(r)}{\gamma^2+E_F}\right|<1 . \qquad (6)$$

Equivalently the linearization is valid[13] for distances $r>r_0$ where r_0 is defined by

$$V(R)-V(r_0)=\gamma^2+E_F . \qquad (7)$$

The solution of Eq. (1) obtained using appropriate boundary conditions $[\lim_{r\to 0} rV(r)\to\mp Z$ for positive or negative charge, respectively, and $\lim_{r\to\infty} V(r)\to 0]$ enables one to calculate the "spatial dielectric function," $\epsilon(r)$, defined by

$$\epsilon(r)=\frac{\mp Z}{rV(r)} . \qquad (8)$$

A wave-vector-dependent dielectric function may be defined as

$$\epsilon(k)=\mp\frac{4\pi Z}{k^2V(k)} , \qquad (9)$$

where $V(\mathbf{k})$ is the Fourier transform of $V(\mathbf{r})$. In the next section we present the numerical results and discussions.

III. NUMERICAL RESULTS AND DISCUSSIONS

The physical parameters used are listed in Table I. The subscript TF is used for quantities in the Thomas-Fermi model neglecting exchange. Table II presents the value of r_0 and the screening radius R obtained for the linearized model [r_0 is obtained using Eq. (7) and R is obtained by using the continuity of the derivative of $V(r)$ at $r=R$]. The results obtained in the TF case (without exchange) are also presented in the same table. Values of the static dielectric function at $r=r_0$ are also given in Table II. It is seen from the table that the region of validity for linearization is smaller for the TFD case when compared to the TF model.

The numerical procedure for solving the nonlinear TFD equation for positive and negative point charges is the same as that for solving the nonlinear TF equation.[2] The nonlinear TFD equation is solved numerically by fourth-order Runge-Kutta method for $Z=\pm1,\pm2,\pm3,\pm4$ in GaAs and GaP. In order to obtain the results for the TF case, we need to put $\gamma=0$ and $E_F=\frac{1}{2}k_F{}^2$ in the input file of the computer program for the TFD case and not mere-

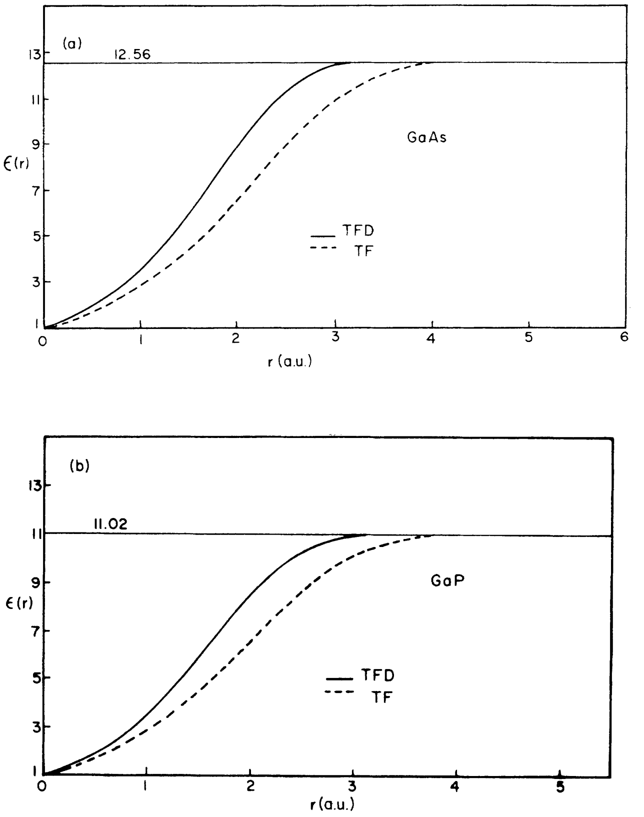

FIG. 2. TF and TFD spatial dielectric functions in the linearized model.

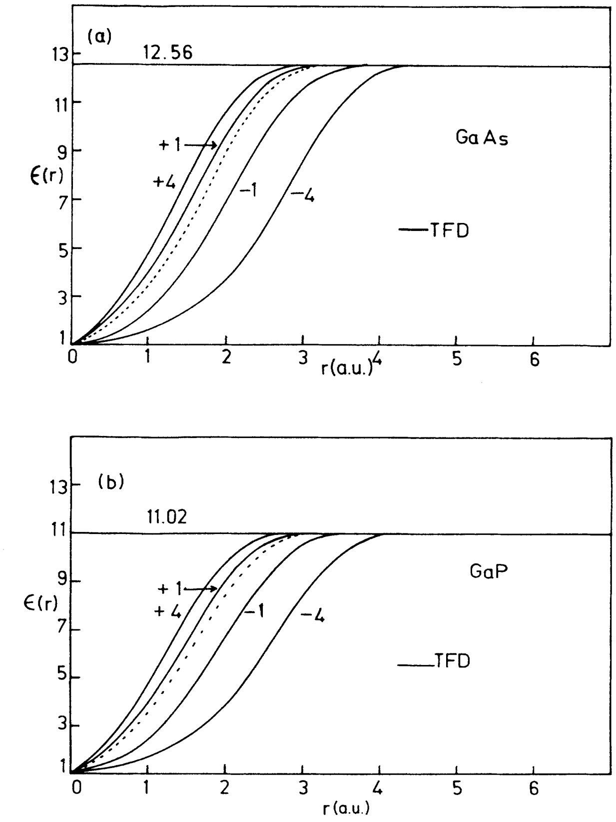

FIG. 3. TFD spatial dielectric functions in the nonlinear regime when $Z=\pm1$ and ±4. The dotted line denotes the Z-independent linearized model.

ly $\gamma = 0$, as was mentioned by Scarfone.[9] Table III reports the screening radii R and Coulomb hole radii R_C obtained from the numerical solution of nonlinear TFD equation. TF values are given in parentheses.

Typical dielectric functions obtained are presented in Figs. 1–6. Figure 1 shows a comparison of the wave-vector-dependent dielectric function obtained in the linear model for both TFD and TF cases. The screening is found to be more effective in the TFD case. Figure 2 shows a similar comparison of the spatial dielectric functions. Figure 3 presents a comparison of the spatial dielectric functions for different Z values (including the linear case specified as $Z = 0$). The results for positive and negative ions fall above and below the linear curve, respectively. Thus, nonlinear screening tends to reduce attractive potentials and enhance repulsive potentials. A comparison of the nonlinear TFD and TF dielectric functions is presented in Figs. 4 and 5. Figure 6 shows a comparison of the results based on the variational method of Ref. 8 and the numerical solution of TF equation. The variational method has not so far been employed for the TFD equation.

When we compare the results obtained on the basis of the statistical models used here with the dielectric functions given by Richardson and Vinsome[14,15] (RV) (a comparison between the TF results and RV have been presented in Refs. 4, 5, and 16), it is seen that the TF results agree better than the TFD results. This indicates that ad-

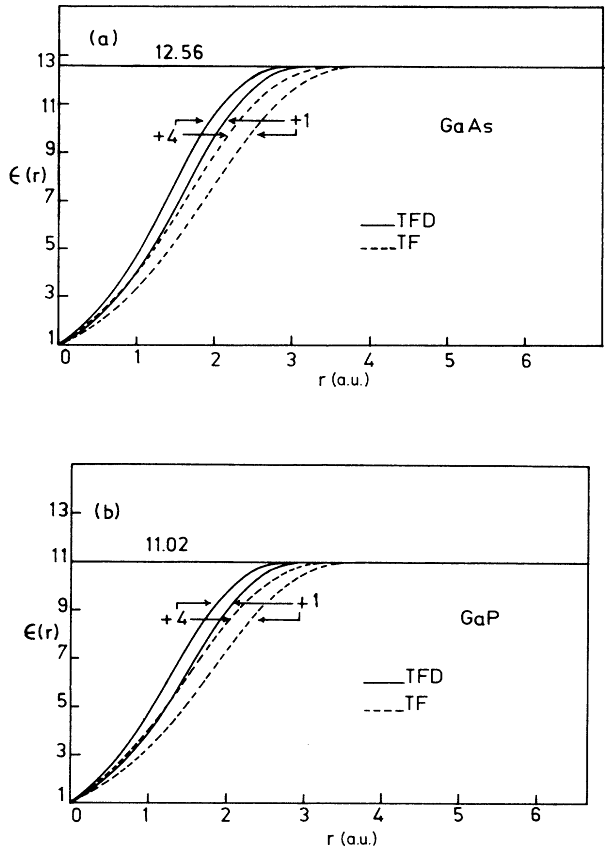

FIG. 4. Comparison of the TF and TFD dielectric functions in the nonlinear regime when $Z = +1$ and $+4$.

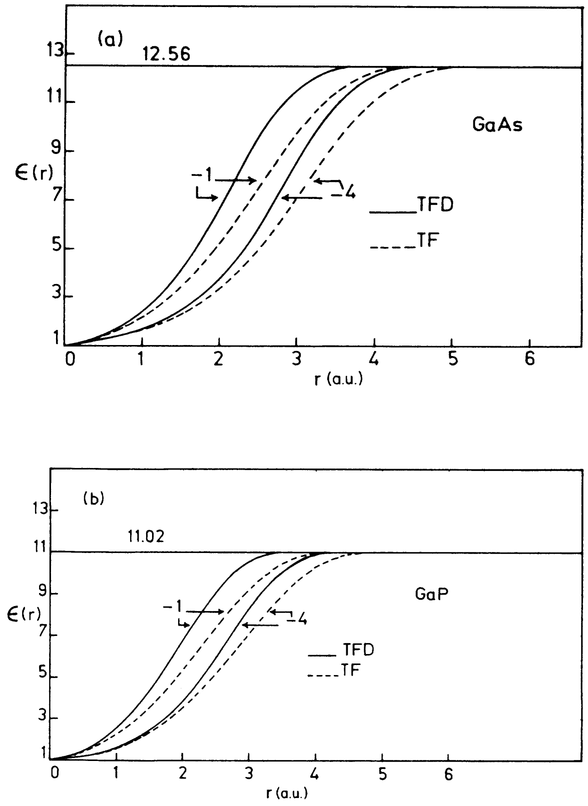

FIG. 5. Comparison of the TF and TFD spatial dielectric functions in the nonlinear regime when $Z = -1$ and -4.

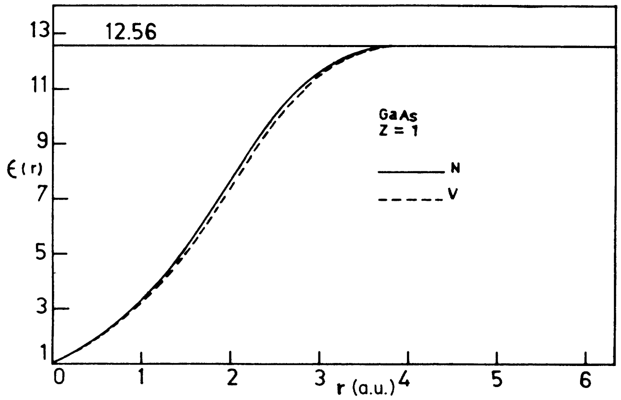

FIG. 6. Comparison of the TF spatial dielectric functions based on the variational approach (V) and numerical solution (N) when $Z = +1$.

ditional effects such as correlation[17] and quantum correction[18] may have to be incorporated, as was pointed out in Ref. 9.

On an examination of the results given in our present work for the two semiconductors, we see that the results are qualitatively similar. This is to be expected, since the models used have not included any of the detailed differences in the band structure of the two materials.

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