Comments

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

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The consequences of an inconsistency in the definition of the Coulomb hole radius given by Scarfone are examined. It is found on solving the nonlinear Thomas-Fermi-Dirac equation numerically that the Coulomb hole radii are different and the screening radii are not much altered when compared with the results of Scarfone. Numerical results for the static dielectric functions are also presented and compared.

In a recent paper Scarfone[1] has used the Thomas-Fermi-Dirac (TFD) statistical theory for obtaining the static dielectric functions for semiconductors. More recently,[2] the same author has discussed the screening of negative impurity ions in semiconductors, revising some part of his earlier work in Ref. 1.

We find an inconsistency in the above works[1,2] in the definition of the Coulomb hole radius R_C. In this Comment we present some of the consequences of this inconsistency.

In the TFD theory, the screened Coulomb potential $V(r)$ due to a negative ion of charge Z (throughout we use atomic units) is obtained by solving the equation (the derivation of which is given in Ref. 1)

$$\nabla^2 V(r) = \begin{cases} \lambda[\gamma + (\gamma^2 + E_F)^{1/2}]^3, & 0 < r \leq R_C \ , \\ \lambda([\gamma + (\gamma^2 + E_F)^{1/2}]^3 - \{\gamma + [(-\gamma)^2 + E_F + V(R) - V(r)]^{1/2}\}^3), & R_C \leq r \leq R \ , \\ 0, & R \leq r < \infty \ , \end{cases} \tag{1}$$

where $\lambda = 2^{7/2}/3\pi$, $\gamma = 1/2^{1/2}\pi$, R is the screening radius, and E_F is the Fermi energy. The Coulomb hole radius is defined in Refs. 1 and 2 by the relation [Eq. (21) of Ref. 1 with equality at $\bullet = R_C$]

$$V(R_C) = E_F + \gamma^2 + V(R) \ . \tag{2}$$

This is inconsistent with the physical requirement that within the Coulomb hole radius, the electron density is a constant equal to $(\lambda/4\pi)[\gamma + (\gamma^2 + E_F)^{1/2}]^3$. If one defines R_C by the equation

$$\{\gamma + [(-\gamma)^2 + E_F + V(R) - V(R_C)]^{1/2}\}^3 = 0 \ , \tag{3}$$

the terms in Eq. (1) are consistent. Equation (3) gives the condition

$$V(R_C) = E_F + V(R) \ , \tag{4}$$

a form identical to the case when exchange is omitted.[3]

With the above modification, we have solved the non-

TABLE I. Listing of screening radii and Coulomb hole radii for nonlinear TFD screening equation for diamond, silicon, and germanium when $Z = -1$, -2, -3, and -4. The values of Ref. 2 are in parentheses.

	Z (a.u.)	Diamond	Silicon	Germanium
Screening radius	-1	2.63(2.63)	3.89(3.91)	4.13(4.14)
R (a.u.)	-2	2.79(2.79)	4.18(4.21)	4.41(4.43)
	-3	2.92(2.92	4.42(4.44)	4.63(4.65)
	-4	3.04(3.04)	4.62(4.64)	4.82(4.85)
Coulomb hole radius	-1	0.69(0.67)	1.42(1.30)	1.37(1.26)
R_C (a.u.)	-2	1.01(0.98)	1.94(1.81)	1.88(1.76)
	-3	1.24(1.21)	2.30(2.17)	2.24(2.10)
	-4	1.43(1.40)	2.60(2.45)	2.52(2.39)

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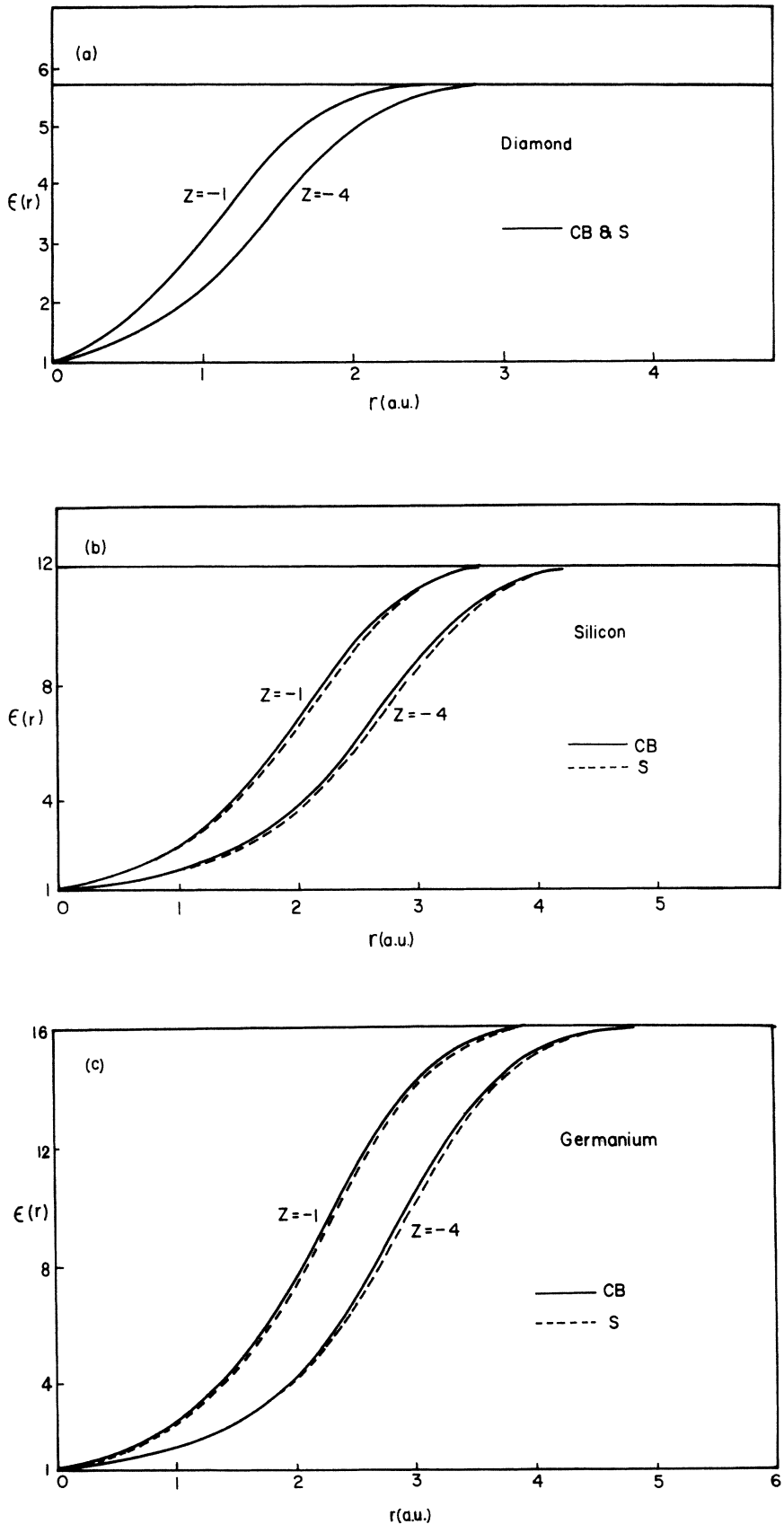

FIG. 1. TFD spatial dielectric function for diamond, silicon, and germanium in the nonlinear regime when $Z = -1$ and -4. ——, present work (CB); – – –, Scarfone (S).

linear TFD equation and found that the Coulomb hole radii are now different as seen in Table I. The screening radii R are not very much altered as would be expected. The accuracy of our numerical method, viz., the fourth-order Runge-Kutta followed by predictor-corrector, has been tested for reproduction of the results in Ref. 2.

We present in Fig. 1 the numerical results obtained for $\epsilon(r)$, the TFD spatial dielectric function, and compare them with those of Scarfone for $Z=-1$ and -4. It is seen that the inconsistency pointed out in the present work has no noticeable consequence on the dielectric function of diamond, while for Si and Ge one can see some difference.

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[2]L. M. Scarfone, Phys. Rev. B **32**, 2653 (1985).

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