Nonlocal contributions to the dielectric screening of point donor impurities in semiconductors

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A Thomas-Fermi theory for dielectric screening in semiconductors is developed in which the effects of exchange and nonlocality are considered. This paper also establishes the region of validity of the linearization and proposes some criteria for the choice of a "single q" in the nonlocal-density approximation. The result shows that the screening radius of a positive point charge is further reduced.

I. INTRODUCTION

Analytical expressions have been found for the dielectric function in **K** space.[1-4] Resta,[5] however, used an **r**-space approach to develop a general theory of screening in semiconductors in which the Thomas-Fermi (TF) screening equation was explicitly solved to obtain a closed analytical expression for the spatial dielectric function $\epsilon(r)$. The main TF equation comes out nonlinear and is then linearized. Recent developments[7-9] have included exchange-correlation and inhomogeneity of the electron gas. These results show a systematic improvements over the TF theory of Resta and have been referred to as the Thomas-Fermi-Dirac[7,8] (TFD) and nonlocal TFD (Ref. 9) theories, respectively. Using the energy-density-functional approach[6,10] a nonlocal TFD equation is obtained.

The nonlocal-density approximation (NLDA) to the exchange-correlation energy functional,[11,12,14] E_{xc}, is chosen in the form of the single **q** approximation of Langreth and Mehl.[13] The present work, however, has not attempted to solve the ensuing nonlinear TFD equation in the nonlocal-density approximation [Eq. (2.14)]. Rather, the emphasis of this work is to demonstrate the contribution of nonlocal effects. Hence Eq. (2.14) is linearized and solved analytically. It should, however, be stated that Eq. (2.14) is the most general form of all the TFD theories. Solution of the nonlinear TFD-NLDA equation will be similar to that recently reported by Scarfone and Enver,[18] although in the local-density approximation comparison of the results obtained in the present work with those in Ref. 18 (especially in the case of $Z=+1$) clearly demonstrates the relative contribution of nonlinearity and nonlocality to the screening of point donor impurities in semiconductors. These results are applied to silicon, to facilitate the comparison. The general solution of the TFD-NLDA is presently being carried out.

II. DIELECTRIC SCREENING

The isotropic spatial dielectric function $\epsilon(r)$ is defined by

$$\epsilon(r)=\frac{-Z}{V(r)r} , \quad r\le R , \tag{2.1}$$

where $V(r)$ is the self-consistent screened potential set up around a static impurity point charge Z placed at the origin. R is the screening radius beyond which $V(r)$ has the Coulomb form screened by the static dielectric constant $\epsilon(0)$,

$$V(r)=\frac{-Z}{r\epsilon(0)} , \quad r\ge R . \tag{2.2}$$

In the presence of the impurity, electrons will take on various values of kinetic energy depending on the potential they "feel." An equilibrium is reached where

$$E_F(r)+V(r)=E_F+V(R) . \tag{2.3}$$

Following the arguments of Langreth and Mehl,[13] we derive a NLDA expression for the Fermi energy E_F of a degenerate electron gas at zero temperature. This is given by

$$E_F(r)=\frac{k_F^2(r)}{2}\left[1-\left[\frac{q}{k_F}\right]^2\right] - \frac{k_F(r)}{\pi}\left[\beta+\left[\frac{q}{k_F}\right]^2\left[2e^{-F}-\tfrac{7}{9}-\tfrac{7}{4}Fe^{-F}\right]\right] \tag{2.4}$$

or

$$E_F(r)=\frac{k_F^2(r)}{2}(1-\delta)-\frac{k_F}{\pi}(\beta+g\delta) , \tag{2.5}$$

where β is the correlation enhancement factor[15] and is given by

$$\beta=1+Bx\ln(1+1/x) , \tag{2.6a}$$

$$x=0.0914/k_F , \tag{2.6b}$$

$$B=0.7734 . \tag{2.6c}$$

The other important wave vector, q, in the system is given by Langreth and Mehl as

$$q(r)=\frac{|\nabla n(r)|}{6n(r)} . \tag{2.7}$$

Other parameters in Eq. (2.4) and (2.5) are

$$k_F(r)=[3\pi^2 n(r)]^{1/3} , \tag{2.8a}$$

$$\delta=\left[\frac{q(r)}{k_F(r)}\right]^2 , \tag{2.8b}$$

$$g=2e^{-F}-\tfrac{7}{9}-\tfrac{7}{4}Fe^{-F} ,$$
$$F=6fq(3\pi/k_F)^{1/2} , \tag{2.8c}$$

and the parameter[13] f is put at 0.15.

In our approximation, we argue that the dependence of the parameters δ and g on position can be neglected. In other words, they do not vary significantly in space within the system. Using the fact that $E_F(r)|_{r-R}=E_F$ one can rewrite Eq. (2.5) as

$$E_F=\frac{k_F^2}{2}(1-\delta)-\frac{k_F}{\pi}(\beta+g\delta) . \tag{2.9}$$

Equations (2.5) and (2.9) are quadratic in $k_F(r)$ and k_F, respectively, and their roots are

$$k_F(r)=\frac{2^{1/2}}{(1-\delta)}\left\{\gamma(\beta+g\delta)+\sqrt{\gamma^2(\beta+g\delta)^2+(1-\delta)[e_F+V(R)-V(r)]}\right\} , \tag{2.10}$$

$$k_F=\frac{2^{1/2}}{(1-\delta)}\left[\gamma(\beta+g\delta)+\sqrt{\gamma^2(\beta+g\delta)^2+(1-\delta)E_F}\right] . \tag{2.11}$$

The perturbed charge density $n(r)$ is then defined in the NLDA theory by

$$n(r)=\frac{2^{3/2}}{3\pi^2(1-\delta)^3}\left\{\gamma(\beta+g\delta)+\sqrt{\gamma^2(\beta+g\delta)^2+(1-\delta)[E_F+V(R)-V(r)]}\right\}^{3/2} \tag{2.12}$$

and the unperturbed ground-state density corresponding to the valence electrons is

$$n_0=\frac{K_F^3}{3\pi^2} \tag{2.13}$$

with k_F defined as in Eq. (2.11). For the sake of self-consistency, the screened impurity potential satisfies the Poisson equation

$$-\nabla^2V(r)=4\pi[n(r)-n_0] . \tag{2.14}$$

Substituting Eqs. (2.12) and (2.13) into this equation, one obtains, using the linearization condition

$$\left|\frac{[V(R)-V(r)](1-\delta)}{\gamma^2(\beta+g\delta)+(1-\delta)E_F}\right|\ll 1 , \tag{2.15}$$

the linearized Poisson equation

$$\nabla^2V(r)=Q^2[V(r)-V(R)] , \tag{2.16}$$

where

$$Q^2=\frac{4k_F^2}{\pi[k_F(1-\delta)-\gamma\sqrt{2}(\beta+g\delta)]} \tag{2.17}$$

The TF theory was originally formulated in connection with dielectric screening in metals where the assumption of continuous states is more nearly satisfied. In the study of insulators and semiconductors, we note that their main difference from metals is the vanishing density in the gap. Actually, real semiconductors always have some impurity states and even very pure samples would still have surface states, all of which give rise to nonvanishing density of gap states.[16]

Therefore, we can use the TF theory to adequately describe incomplete impurity screening in semiconductors provided the correct boundary conditions are used. The linearized Poisson equation is solved using the following boundary conditions:

$$\lim_{r\to 0}[rV(r)]=\lim_{r\to 0}[rV_0(r)]=-Z , \tag{2.18}$$

$$V(R)=\frac{V_0(R)}{\epsilon(0)}=\frac{-Z}{\epsilon(0)R} , \tag{2.19}$$

where

$$V_0(r)=-\frac{Z}{r} . \tag{2.20}$$

The solution of Eq. (2.16) obtained using these boundary conditions is

$$V(r)=\frac{-Z}{r}\frac{\sinh[Q(R-r)]}{\sinh[QR]}+V(R) . \tag{2.21}$$

Imposing the continuity condition on the electric field at $r=R$, one obtains a transcendental equation

$$\sinh[QR]=QR\epsilon(0) \tag{2.22}$$

from which the screening radius is obtained. A closed analytical expression for the spatial dielectric function is obtained using Eqs. (2.1) and (2.21),

$$\epsilon(r)=\begin{cases}\dfrac{\epsilon(0)QR}{\sinh[Q(R-r)]+QR}, & r\le R\\ \epsilon(0), & r\ge R .\end{cases} \tag{2.23}$$

The major difference between this treatment and the earlier ones due to Resta[5] and Scarfone[8] is that it has the effects of both exchange-correlation and inhomogeneity incorporated.

III. RESULTS AND DISCUSSION

The result obtained in the preceding section is applied to study the screening characteristics of the group-IV semiconducting elements, specifically, for silicon. We consider four possible cases: (i) $\gamma=0$, $\delta=0$, this is equivalent to the TF-LDA theory; (ii) $\gamma=0$, $\delta\neq 0$, the

TABLE I. Results for silicon. Here, the nearest-neighbor distance $a=4.44$ a.u., the static dielectric constant $\epsilon(0)=11.94$, and the valence Fermi momentum $K_F=0.96$. Wave vector q in Eq. (2.7) corresponds to the 3s orbital in the Si atom (Ref. 17).

	TF-LDA	TF-NLDA	TFD-LDA[a]	TFD-NLDA[a]
Fermi energy	E_F 0.461	0.446	0.155 (0.100)	0.263 (0.167)
	Q 1.106	1.315	1.352 (1.417)	1.551 (1.740)
Screening radius	R 4.275	3.593	3.495 (3.335)	3.048 (3.716)
$r(z=1)$	0.849	0.932	1.098 (1.148)	1.015 (1.033)
Region of validity				
$R-r$	3.426	2.661	2.397 (2.187)	2.033 (1.683)
$r(z=2)$	1.178	1.240	1.420 (1.464)	1.300 (1.298)
$R-r$	3.097	2.353	2.075 (1.871)	1.748 (1.418)
$r(z=3)$	1.393	1.436	1.620 (1.659)	1.477 (1.460)
$R-r$	2.882	2.157	1.875 (1.676)	1.571 (1.256)
$r(z=4)$	1.554	1.580	1.766 (1.801)	1.606 (1.577)
$R-r$	2.721	2.013	1.729 (1.534)	1.442 (1.139)

[a] Results obtained when the correlation effect is included are shown in parentheses.

TF-NLDA theory; (iii) $\gamma\neq 0$, $\delta=0$, the TFD-LDA theory; (iv) $\gamma\neq 0$, $\delta\neq 0$, the TFD-NLDA theory.

Using the linearization condition of Eq. (2.15), regions of validity are established for these four cases and the results are shown in Table I, along with the values of Q, E_F, and R for each case (all results are for $Z=+1$). Unlike our earlier work where the effect of correlation was left out, we here show the results arising from inclusion of correlation (these are put in parentheses in the table). We observe that the inclusion of correlation further decreases the screening radii and increases the regions of validity beyond the ones previously obtained.

In this work our emphasis has been on nonlocality. Nonlinear effects have been shown also to lead to better screening of impurities in semiconductors.[8] A combined effect of nonlinearity, nonlocality, and full exchange-correlation is being investigated. Furthermore, dielectric function obtained from this model is to be applied to study electron-hole interaction in exciton problems. In all these calculations, it should be noted that the Fermi surface of silicon is not spherical (as in a free-electron gas model). We have determined the appropriate q using the density corresponding to the 3s orbital. In an effort to keep the calculations simple, we have used functions simpler than the Hartree-Fock (HF) functions. For this purpose we made use of the single-exponential function to describe an atomic orbital in the fashion prescribed by the self-consistent-field (SCF) method.[17] The values of q obtained using the SCF method agree with those obtained from the HF atomic orbitals by Langreth and Mehl[13] in the case of beryllium.

Finally, it is noted that the effect of nonlocality on the spatial dielectric functions is quite significant and constitutes our major results. The TFD-NLDA is more effective at reducing attractive potentials than either the linear or nonlinear TFD theories of Scarfone.[8] It should, however, be stated here that the value obtained by Scarfone and Enver[18] for the screening radius in the nonlinear TFD regime is very close to that obtained here in the nonlocal TFD regime for the monovalent impurities for which the linear approximation is most appropriate. From these two results, one observes that both nonlinearity and nonlocality tend to reduce the range of the attractive potential of the impurity.

[1]D. R. Penn, Phys. Rev. **128**, 2093 (1962).
[2]G. Srinivasan, Phys. Rev. **178**, 1244 (1969).
[3]J. P. Walter and M. L. Cohen, Phys. Rev. B **2**, 1621 (1976).
[4]F. Bassani, G. Iodonisi, and B. Preziosi, Rep. Prog. Phys. **37**, 1099 (1974).
[5]R. Resta, Phys. Rev. B **16**, 2717 (1977).
[6]W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
[7]P. Scavinsky, Phys. Rev. B **28**, 6076 (1983).
[8]L. M. Scarfone, Phys. Rev. B **29**, 3259 (1984).
[9]S. B. Elegba and A. I. Amali, J. Phys. C **19**, L169 (1986).
[10]P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).
[11]O. Gunnarsson, M. Jonson, and B. I. Lundqvist, Solid State Commun. **24**, 765 (1977).
[12]J. A. Alonso and L. A. Girifalco, J. Phys. Chem. Solids **39**, 79 (1978); Phys. Rev. B **17**, 3735 (1978).
[13]D. C. Langreth and M. J. Mehl, Phys. Rev. Lett. **47**, 456 (1981); Phys. Rev. B **28**, 1809 (1983); **29**, 2310 (1984).
[14]D. C. Langreth and J. P. Perdew, Phys. Rev. B **15**, 2884 (1977).
[15]L. Hedin and B. I. Lundqvist, J. Phys. C **4**, 2064 (1971).
[16]C. O. Almbladh and U. Von Barth (unpublished).
[17]E. Clementi and D. L. Raimondi, J. Chem. Phys. **38**, 2686 (1961).
[18]L. M. Scarfone and A. Enver, Phys. Rev. B **43**, 2272 (1991).