Thomas-Fermi-Dirac dielectric response of a semiconductor

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The purpose of the present paper is the investigation of the importance of exchange in the dielectric response of a semiconductor. It is shown that within the framework of the linearized Thomas-Fermi-Dirac theory the spatial dielectric function of a semiconductor can be obtained in a very simple analytical form that differs from the form obtainable from the linearized Thomas-Fermi (TF) theory only by different values of the constants appearing in it. The main conclusion is that introduction of exchange results in a contraction of the TF screening radius beyond which the screening of a positive point charge by the valence electrons is complete.

I. INTRODUCTION

The spatial dielectric function $\bar{\epsilon}(\vec{r})$ of a (pure) semiconductor, such as Si, describes the response of the valence electrons to a (point) charge placed into the medium. The response consists of a rearrangement of the valence electrons that, in turn, leads to the shielding of the potential of the charge. Until a few years ago, the calculation of the spatial dielectric function involved several steps. First, the wave-vector-dependent dielectric function $\epsilon(\vec{k})$ is obtained (usually by large-scale computations) in a given direction[1] in $\vec{k}$ space in numerical form. Second, $\epsilon(\vec{k})$ is approximated by some conveniently chosen analytical function. Third, the analytical function selected is Fourier transformed to obtain the corresponding spatial dielectric function $\bar{\epsilon}(\vec{r})$. As an illustration of this procedure, the calculations (for Si) of Srinivasan[2] are quoted.

A few years ago, however, another approach for calculating $\bar{\epsilon}(|\vec{r}|)$ became available when Resta[3] had formulated a Thomas-Fermi screening theory for obtaining an isotropic $\bar{\epsilon}(r)$. The attractiveness of this approach lies in the fact that all calculations are carried out in direct space instead of in reciprocal space. By linearizing[4] the TF equation for the potential (energy) of the charge, Resta[3] was able to solve it in a closed form and derive a quite simple analytical expression for $\bar{\epsilon}(r)$.

The TF theory of atoms and ions[5] is, however, beset with a deficiency. This deficiency consists in the neglect of the exchange among the electrons. This shortcoming of the TF theory has been remedied by Dirac,[6] leading to the so-called TFD model of atoms and ions.[7] One of the manifestations of the introduction of exchange is a contraction of the radius of an ion. For instance, the Rb^+ ion has a radius of 5.91 (in a.u.) in the TF model,[8] while its radius in the TFD model[9] is 3.44 (in a.u.). On this basis, one also expects that Resta's TF screening radius, beyond which the screening of a positive (point) charge is complete, will also be reduced when calculated in the TFD framework. The present work confirms this expectation and leads to a modified spatial dielectric function. In what follows atomic units[10] will be used and the semiconductor silicon will be considered as an example.

II. THEORY

The (isotropic[11]) spatial dielectric function $\bar{\epsilon}(r)$ is defined by

$$U(r) = -\frac{Z}{\bar{\epsilon}(r) r} \ , \tag{1}$$

where $U(r)$ is the potential (energy[12]) of the (point[13]) charge Z, and r is the distance from it.

Poisson's equation, for the potential $U(r)$ of the charge embedded in a semiconductor is given by

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

In Eq. (2),

$$n_0 = k_F^3/3\pi^2 \tag{3}$$

is the concentration of the valence electrons,[14] while, in the TFD theory,

$$n(r) = (2^{3/2}/3\pi^2)\{a + [E_0 - U(r) + a^2]^{1/2}\}^3 \tag{4}$$

is the electron density at a distance r from the charge.[15] In Eq. (3), k_F denotes the valence Fermi momentum, which is related to the valence Fermi energy E_F by

$$E_F = k_F^2/2 \ . \tag{5}$$

In Eq. (4), a denotes the constant

$$a = (2^{1/2}\pi)^{-1} \ , \tag{6}$$

while E_0 is the maximum energy available to an electron. This quantity can be written as

$$E_0 = E_F + A \ , \tag{7}$$

where the constant A will be determined later.

Substituting Eq. (4) into Eq. (2), and linearizing[16] the resulting equation in terms of the quantity

$$x = \frac{A - U(r) + a^2}{E_F} \ , \tag{8}$$

one obtains

$$\nabla^2 U(r) = Q^2 [U(r) - C] \ . \tag{9}$$

In Eq. (9), Q denotes the constant

$$Q^2 = (2^{7/2}/3\pi)(\tfrac{3}{2}E_F^{1/2} + 3a + \tfrac{3}{2}a^2 E_F^{-1/2}) \ , \tag{10}$$

while C is another constant, defined by

$$C = A + B/Q^2 \ , \tag{11}$$

with B given by

$$B = (2^{7/2}/3\pi)(3aE_F + \tfrac{9}{2}a^2 E_F^{1/2} + 4a^3 + \tfrac{3}{2}a^4 E_F^{-1/2}) \ . \tag{12}$$

The constant A in Eq. (7) is determined by the requirement that the charge be completely screened at a distance R

from the charge. This requirement is stated by

$$n(R)=n_0 \ , \tag{13}$$

that, upon the linearization of Eq. (4) in terms of the quantity defined in Eq. (8), leads to

$$A=U(R)-B/Q^2 \ . \tag{14}$$

Substituting Eq. (14) into Eq. (11) one finds that

$$C=U(R) \ . \tag{15}$$

Considering Eq. (5), and introducing the constant

$$q=(4k_F/\pi)^{1/2} \ , \tag{16}$$

Eq. (10) is brought to the form

$$Q^2=q^2\left[1+\frac{2^{7/2}}{\pi}aq^{-2}+\frac{2^5}{\pi^2}a^2q^{-4}\right] \ . \tag{17}$$

It is seen from Eq. (17) that, upon putting a equal to zero, one recovers Resta's TF result.[3] To put it another way, the terms in a and a^2 in the square brackets in Eq. (17) represent the corrections to the TF result due to the introduction of exchange.

The solution of Eq. (9) is sought in the form

$$U(r)=-\frac{Z}{r}(\alpha e^{Qr}+\beta e^{-Qr})+C \ , \tag{18}$$

where C is given by Eq. (15). The solution should obey a boundary condition at $r=0$, and at $r=R$. The first boundary condition is stated by

$$\lim_{r\to 0}[rU(r)]=-Z \ , \tag{19}$$

while the second boundary condition is stated by

$$U(R)=-\frac{Z}{\epsilon(0)R} \ , \tag{20}$$

where $\epsilon(0)$ is the static dielectric constant of the semiconductor.

Imposing Eq. (19) on Eq. (18), one finds that

$$\beta=1-\alpha \ . \tag{21}$$

Imposing Eq. (20) on Eq. (18), and considering Eq. (21), one obtains

$$\alpha=-\frac{e^{-QR}}{2\sinh(QR)} \ . \tag{22}$$

Using Eqs. (20)–(22), Eq. (18) assumes the form

$$U(r)=-\frac{Z}{r}\frac{\sinh[Q(R-r)]}{\sinh(QR)}-\frac{Z}{\epsilon(0)R} \ . \tag{23}$$

The screening radius R, in Eq. (23), is determined from the condition that the electric field be continuous at $r=R$. This condition is expressed by

$$\left[\frac{d}{dr}\left(-\frac{Z}{\epsilon(0)r}\right)\right]_{r=R}=\left[\frac{d}{dr}U(r)\right]_{r=R} \tag{24}$$

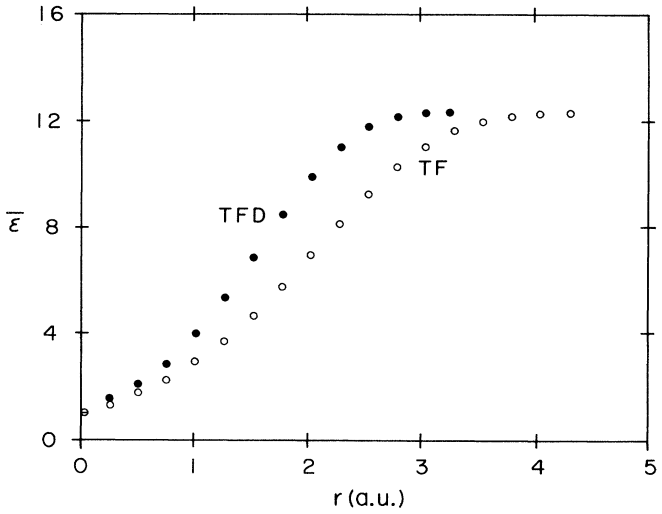

FIG. 1. Dependence of $\bar{\epsilon}(r)$ on r as obtained from the linearized TF and TFD approaches.

and leads to

$$\frac{\sinh(QR)}{QR}=\epsilon(0) \ . \tag{25}$$

Finally, from Eqs. (1) and (23), upon consideration of Eq. (25), the spatial dielectric function can be obtained in the form

$$\bar{\epsilon}(r)=\frac{\epsilon(0)QR}{\sinh[Q(R-r)]+Qr} \ . \tag{26}$$

III. DISCUSSION

Equation (26) for $\bar{\epsilon}(r)$ is of the same form as that obtained by Resta.[3] The only difference is that in Resta's formula for $\bar{\epsilon}(r)$ the quantity Q [defined in Eq. (17)] is replaced by the quantity q [defined in Eq. (16)]. For silicon, these quantities have the values of $Q=1.47$ a.u. and $q=1.10$ a.u., respectively. When the screening radius is determined [from Eq. (25)],[17] one finds that it has the value of $R=3.22$ a.u., which is compared with Resta's TF value of 4.28 a.u. It is seen that the contraction of the screening radius is significant. The ratio of R(TFD)/R(TF) is 0.75. This value may be compared with TFD Rb^+ radius/TF Rb^+ radius which is 0.58.

The behavior of $\bar{\epsilon}(r)$ as a function of r is illustrated in Fig. 1, both for the TF and for the TFD cases. Considering that in silicon the nearest-neighbor distance is 4.44 a.u., it is seen that in the TF case the screening of the charge is not complete until very close to the nearest-neighbor distance while in the TFD case the screening is complete at about $\frac{3}{4}$ of the nearest-neighbor distance.

[1]Calculations by J. P. Walter and M. L. Cohen [Phys. Rev. B 2, 1621 (1970)] show that, for Si and Ge, $\epsilon(\vec{k})$ is nearly isotropic.
[2]G. Srinivasan, Phys. Rev. 178, 1244 (1969).
[3]R. Resta, Phys. Rev. B 16, 2717 (1977).
[4]The consequences of the linearization have been investigated by P. Csavinszky [Phys. Rev. B 21, 632 (1980)] who concluded that, for a charge $Z=+1$ (in a.u.), for instance, in diamond, silicon, and germanium, the linearized TF equation loses its validity at a

distance from the charge which is about $\frac{1}{5}$ of the screening radius. The use of the linearized equation for all values of the independent variable can, however, be justified as an extrapolation dictated by expediency.

[5]For a comprehensive review of the subject, see P. Gombás, *Die statistische Theorie des Atoms und ihre Anwendungen* (Springer, Wien, 1949), p. 30ff.

[6]P. A. M. Dirac, Proc. Cambridge Philos. Soc. 26, 376 (1930).

[7]See Ref. 5, p. 76ff.

[8]See p. 57 of Ref. 5.

[9]See p. 87 of Ref. 5.

[10]We use the following units: Magnitude of the electron charge = 1, Planck's constant divided by $2\pi = 1$, electron mass = 1, and unit of length = bohr.

[11]From now on the isotropic spatial dielectric function will simply be referred to as the spatial dielectric function.

[12]From now on the potential energy will simply be referred to as the potential.

[13]From now on the point charge will simply be referred to as the charge.

[14]To obtain n_0, one considers that the silicon unit cube contains eight silicon atoms and each silicon atom contributes four valence electrons.

[15]Equation (4) is in the notation of N. H. March [Adv. Phys. 6, 5 (1957)] with the potential $V(r)$ replaced by the potential energy $U(r)$.

[16]The consequences of the linearization of the TFD equation are not expected to be materially different from those of the TF equation. See Ref. 4 in this regard.

[17]Using the value of $\epsilon(0) = 11.94$.