Thomas-Fermi dielectric screening in semiconductors

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(Received 22 September 1978)

The present note investigates the range of validity of Resta's linearized Thomas-Fermi (TF) approach to dielectric screening in semiconductors.

I. INTRODUCTION

In a recent paper, Resta[1] has developed a Thomas-Fermi (TF) theory of the screening of point impurity charges in semiconductors. By linearizing the TF equation, Resta was able to solve it in a closed form and then use the solution to obtain an analytical expression for the spatial dielectric function $\epsilon(|\vec{r}|)$ for the semiconductors diamond, silicon, and germanium. An attractive feature of Resta's theory lies in the fact that ϵ is obtained from $\vec{r}$-space considerations, thereby avoiding the need for the Fourier transform of the corresponding $\vec{k}$-space quantity.

In another recent paper, Cornolti and Resta[2] gave, for the first time, numerical solutions of the nonlinear TF equation for different values of the impurity charge Z in the same semiconductors. The nonlinear results, while not invalidating the linear theory, showed important deviations from the linear results, namely, a more effective screening for positive values of Z.

In view of the fact that the analytical feature of the linear theory makes it attractive for applications, it is important to investigate the range of validity of the linearized TF equation. This is accomplished in the present note for different positive values of Z.

II. DISCUSSION

Resta's basic equation, in atomic units ($\hbar=1$, $e^2=1$, $m_e=1$), is

$$-\nabla^2 V(r)=(2^{7/2}/3\pi)\{[E_F+A-V(r)]^{3/2}-E_F^{3/2}\}, \quad (1)$$

where $V(r)$ is the screened (point) donor-ion potential,

$$E_F=\tfrac{1}{2}k_F^2 \quad (2)$$

is the Fermi energy expressed in terms of the Fermi momentum k_F, and A is a constant.

The simplifying feature of Resta's theory is the linearization of Eq. (1), which involves a binomial expansion in terms of the quantity

$$x=[A-V(r)]/E_F. \quad (3)$$

With the expression obtained by Resta for $[A-V(r)]$, the criterion for the validity of the binomial expansion can be written as

$$x^2=\left(\frac{Z}{r}\frac{\sinh q(R-r)}{\sinh qR}\right)^2 E_F^{-2}<1, \quad (4)$$

where

$$q=(4k_F/\pi)^{1/2}, \quad (5)$$

$Z=1, 2, 3, \ldots$, and R is a screening radius, whose value[2] (in a. u.) for diamond, silicon, and germanium is 2.76, 4.28, and 4.54.

Using Eq. (2), Eq. (4) may be simplified to

$$\frac{Z}{r}\frac{\sinh q(R-r)}{\sinh qR}<\tfrac{1}{2}k_F^2. \quad (6)$$

It is obvious from Eq. (6) that, at some value of r (say r_0) in the $0<r<R$ range, the inequality will break down.

For a singly charged ($Z=1$) donor ion (using Resta's values for q, R, and k_F), the inequality in Eq. (6) becomes an equality at the r_0 values listed in column 2 of Table I. In view of this fact, use of the linearized form of Eq. (1) in the region of $r<r_0$ is, strictly speaking, not justified. The fact that a linearized equation loses validity in some range of the independent variable is, of course, a common feature of all linearized theories. The use of the linearized equation for all values of the independent variable can perhaps be justified as an extrapolation dictated by expediency.

TABLE I. Quantities pertinent to the linearization of Eq. (1) when $Z=1$.

Semiconductor	r_0 (a.u.)	r_0'	$\bar{\epsilon}(r_0)$	$[\bar{\epsilon}(r_0)/\epsilon(0)]$ (100%)	r_0/R
Diamond	0.48	0.16	1.82	31.9	0.17
Silicon	0.85	0.19	2.48	20.8	0.20
Germanium	0.90	0.19	2.58	16.1	0.20

TABLE II. Quantities pertinent to the linearization of Eq. (1) when $Z=2$.

Semiconductor	r_0 (a.u.)	r_0'	$\bar{\epsilon}(r_0)$	$[\bar{\epsilon}(r_0)/\epsilon(0)]$ (100%)	r_0/R
Diamond	0.71	0.24	2.36	41.4	0.26
Silicon	1.18	0.27	3.42	28.6	0.28
Germanium	1.24	0.27	3.61	22.5	0.27

The numerical values of r_0, as listed in Table I, do not say much in themselves. It is more interesting to find out just how large r_0 is on the scale of the crystal lattice. Denoting the nearest-neighbor distance by a, the "reduced" cutoff radii,

$$r_0'=r_0/a\,, \tag{7}$$

have been calculated and listed in column 3 of Table I. Inspection of the r_0' values shows that, on the lattice scale, they are not negligible. For this reason, it is of interest to find out what the $\bar{\epsilon}(r_0)$ values are. This can be done from Resta's expression of

$$\bar{\epsilon}(r)=\frac{\epsilon(0)qR}{\sinh q(R-r)+qr}\,, \tag{8}$$

where $\epsilon(0)$ is the static dielectric constant of the semiconductor. Using Resta's values for $\epsilon(0)$, the values of $\bar{\epsilon}(r_0)$, as calculated from Eq. (8), are listed in column 4 of Table I. Again, the numerical values by themselves, do not say much. It is of more interest to find out what percentage of the relevant static dielectric constant is represented by the $\bar{\epsilon}(r_0)$ values. These quantities are listed in column 5 of Table I. Inspection of the $[\bar{\epsilon}(r_0)/\epsilon(0)]$ (100%) values show that a significant percentage of the $\epsilon(0)$ values is already attained at $r=r_0$. Recalling that the screening of the positive point charge is confined to the interval $0\leq r\leq R$, another quantity of interest is the ratio of r_0/R. This is shown in column 6 of Table I. Inspection of these values shows that the linearized TF equation is not valid for a space region of about $\frac{1}{5}$ of the screening radius.

So far, the case of $Z=1$ has been dealt with. It is of interest to find out just what the situation is when one deals with a doubly charged donor ion. Using $Z=2$ in Eq. (6), quantities similar to those in Table I have been calculated and listed in Table II. It is seen that the r_0 values are larger for $Z=2$ than for $Z=1$. As a result, all other quantities in Table II are shifted in magnitude relative to those in Table I. It is noteworthy, as inspection of column 6 of Table II shows, that the linearized TF equation is not valid for a space region which is about $\frac{1}{4}$ of the screening radius.

There appears to be no doubt that the $Z=3$, 4... cases are even less favorable. This is, of course, not surprising, since it is known[2,3] that linearization is exact only for a vanishingly small charge.

III. CONCLUSION

For highly charged impurities, known to exist in semiconductors, the nonlinear theory of screening appears to be preferable over the linear theory of screening. This conclusion is in agreement with the findings of Cornolti and Resta,[2] whose results show that the larger the value of Z, the greater the discrepancy between the linear and nonlinear spatial dielectric functions. This is in agreement with the findings in this paper, namely, that the larger the value of Z, the less adequate the process of linearization.

Finally, it is mentioned that the results of the nonlinear theory[2] for negative ions are also better than those of the linear theory.[1] Undoubtedly, this is also due to the same reasons as those discussed above in connection with positive ions. The case of negative ions, however, has not been touched upon in this paper since the presence of the Coulomb hole adds a complicating aspect but no additional insight.

[1]R. Resta, Phys. Rev. B 16, 2717 (1977).
[2]F. Cornolti and R. Resta, Phys. Rev. B 17, 3239 (1978).
[3]W. Kohn, Phys. Rev. 105, 509 (1957).