PHYSICAL REVIEW B VOLUME 24, NUMBER 8 15 OCTOBER 1981

Nonlinear screening of positive point charges in diamond, silicon, and germanium

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(Received 9 March 1981)

In the present paper we have formulated a variational principle for obtaining approximate analytical solutions of a nonlinear differential equation established by Cornolti and Resta for the potentials of positive point charges embedded in pure diamond, silicon, and germanium. We have considered the cases of charges $Z=+1,\ +2,\ +3,\ +4$ (in atomic units) in these semiconductors, while Cornolti and Resta considered the cases of $Z=+1,\ +4$. We find that our approximate analytical results for the spatial dielectric functions of diamond, silicon, and germanium, depending on Z, are in excellent agreement with the numerical results of Cornolti and Resta, who have presented their results in the form of graphs.

I. INTRODUCTION

The spatial dielectric function of a semiconductor is of importance in a variety of problems.[1] In general, the calculation of this quantity proceeds as follows. First, the wave-vector-dependent dielectric function $\epsilon(\vec{k})$ is obtained in a given direction in $\vec{k}$ space, in tabular form. Second, this quantity is approximated by some conveniently chosen analytical function. Third, the analytical function selected is used in a Fourier inversion to obtain the corresponding spatial dielectric function $\bar{\epsilon}(\vec{r})$.

Recently, Resta[2] has formulated a Thomas-Fermi (TF) approach for obtaining an isotropic $\bar{\epsilon}(r)$. The attractive feature of this approach lies in the fact that all considerations are made in direct space instead of in reciprocal space. The linearized version of Resta's theory[2] leads to a quite simple analytical formula for $\bar{\epsilon}(r)$. Resta's result,[2] for the potential energy[3] of a screened positive point charge Z, can be stated by

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

where the spatial dielectric function $\bar{\epsilon}_l(r)$, associated with the linearized theory, is given by

$$\bar{\epsilon}_l(r)=\begin{cases}\epsilon(0)qR_l/[\sinh q(R_l-r)+qr], & r\le R_l\\ \epsilon(0), & r\ge R_l\ .\end{cases} \tag{2}$$

In Eq. (2), $\epsilon(0)$ is the static dielectric constant of the semiconductor, R_l is a screening radius, and q is a constant defined by

$$q=(4k_F/\pi)^{1/2}\ , \tag{3}$$

where k_F stands for the valence Fermi momemtum. The above quantities, for diamond, silicon, and germanium, have been tabulated by Resta.[2,4]

In another paper, Cornolti and Resta[5] have solved numerically Resta's nonlinear TF equation[2] for the potential of point ions, and presented graphical results for $\bar{\epsilon}_n(r)$, the spatial dielectric function associated with the nonlinear theory, for point charges $Z=\pm1, \pm4$ in pure diamond, silicon, and germanium. Their graphs of $\bar{\epsilon}_n(r)$ versus r show important deviations from the $Z=0$ linearized results,[6] i.e., from the graph of $\bar{\epsilon}_l(r)$ versus r. Some aspects of the consequences of the linearization have been discussed by Csavinszky.[7]

The goal of the present work is to obtain $\bar{\epsilon}_n(r)$ analytically for point charges, $Z=+1,\ +2,\ +3,\ +4$ in pure diamond, silicon, and germanium. This we accomplish by obtaining an approximate solution of the nonlinear TF equation[2,5] by an equivalent variational principle. In what follows, as in the preceding equations, all quantities are written using atomic units.[8]

II. THEORY

The nonlinear TF equation, solved by Cornolti and Resta[5] is

$$\nabla^2 V(r)=\begin{cases} a\{E_F^{3/2}-[E_F+A-V(r)]^{3/2}\}, & r\le R_n \\ 0, & r\ge R_n \end{cases} \tag{4}$$

where a and A are constants, defined by

$$a=2^{7/2}/3\pi \tag{5}$$

and

$$A=V(R_n)\,, \tag{6}$$

respectively. In Eq. (4), V is the potential of the point charge embedded into the pure semiconductor, and E_F denotes the valence Fermi energy which is related to the valence Fermi momentum k_F by

$$E_F=k_F^2/2\,. \tag{7}$$

In Eq. (6), R_n denotes a Z-dependent screening radius beyond which the screened potential due to a positive point charge Z is given[5] by

$$V(r)=-\frac{Z}{\epsilon(0)r} \quad r\ge R_n\,. \tag{8}$$

Our goal is to solve Eq. (4) in an approximate analytical form by an equivalent variational principle. For this reason, we shall consider the (first) variation of the integral

$$I=\int_0^{R_n} F(\psi,\psi',r)dr\,, \tag{9}$$

where the variable $\psi(r)$, its derivative $\psi'(r)$, and the function $F(\psi',\psi,r)$ will be discussed later. We note here that, in the terminology of Courant and Hilbert,[9] our variational problem is of the "variable domain" type since not only the function $\psi(r)$ but also the upper limit R_n is a variable. The (first) variation of the integral I is given[9] by

$$\delta I=\int_0^{R_n}\left[-\frac{d}{dr}\frac{\partial F}{\partial\psi'}+\frac{\partial F}{\partial\psi}\right]\delta\psi\,dr + \frac{\partial F}{\partial\psi'}\delta\psi\Big|_{r=R_n}-\frac{\partial F}{\partial\psi'}\delta\psi\Big|_{r=0}+F\Big|_{r=R_n}\delta R_n\,, \tag{10}$$

where the second, third, and fourth terms are due to the variation of the domain.

We also note here that F must be so chosen that, upon its substitution into the Euler-Lagrange equation

$$-\frac{d}{dr}\frac{\partial F}{\partial\psi'}+\frac{\partial F}{\partial\psi}=0\,, \tag{11}$$

one recovers Eq. (4). In addition, we must also find a quantity G such that

$$\delta G=\left[-\frac{\partial F}{\partial\psi'}\delta\psi\Big|_{r=R_n}\right]-\left[-\frac{\partial F}{\partial\psi'}\delta\psi\Big|_{r=0}\right]-F\Big|_{r=R_n}\delta R_n\,. \tag{12}$$

With F and G chosen according to the above requirements, our variational principle can be stated by

$$\delta\left[\int_0^{R_n} F\,dr+G\right]=0\,. \tag{13}$$

We shall first find an expression for F. Let us introduce the function

$$\psi(r)=r[V(r)-A]\,, \tag{14}$$

which, upon consideration of Eqs. (6)–(8) becomes, for $r\ge R_n$,

$$\psi(r)=[-Z/\epsilon(0)](1-r/R_n)\,. \tag{15}$$

We note here that for $r\ge R_n$ the following relations are satisfied:

$$\psi(R_n)=0\,, \tag{16}$$

$$\delta\psi\Big|_{r=R_n}=-\frac{Z}{\epsilon(0)}\left[-r\delta\left[\frac{1}{R_n}\right]\right]_{r=R_n}=-\frac{Z}{\epsilon(0)}\frac{\delta R_n}{R_n}\,, \tag{17}$$

$$\psi'\Big|_{r=R_n}=\frac{Z}{\epsilon(0)R_n}\,. \tag{18}$$

Equation (16) follows from Eqs. (6) and (14). Equation (17) follows from Eq. (15) upon consideration of $\delta(1/R_n)=-\delta R_n/R_n^2$. Equation (18) follows from Eq. (15).

Using Eq. (15), one finds that Eq. (4) can be brought to the form

$$\psi''-a\left[rE_F^{3/2}-r\left[E_F-\frac{\psi}{r}\right]^{3/2}\right]=0,\quad r\le R_n\,. \tag{19}$$

Choosing the integrand F in Eq. (13) as

$$F=-\tfrac{1}{2}(\psi')^2-a\left[rE_F^{3/2}\psi+\tfrac{2}{5}r^2\left[E_F-\frac{\psi}{r}\right]^{5/2}\right], \tag{20}$$

differentiation shows that Eq. (11) becomes

$$-\frac{d}{dr}\frac{\partial F}{\partial \psi'}+\frac{\partial F}{\partial \psi}=\psi''-a\left[rE_F^{3/2}-r\left[E_F-\frac{\psi}{r}\right]^{3/2}\right]=0\ , \tag{21}$$

which is recognized as Eq. (19).[10]

We shall turn now to the task of finding an expression for G. For this purpose Eq. (12), with the aid of Eqs. (17) and (18), is written as

$$\delta G=\psi'\Big|_{r=R_n}\delta\psi\Big|_{r=R_n}-F\Big|_{r=R_n}\delta R_n\ . \tag{22}$$

We note here that in arriving at this expression, Eq. (20) has been considered, from which

$$-\frac{\partial F}{\partial \psi'}=\psi'\ . \tag{23}$$

We also note here that the term $-(\delta F/\delta\psi')\,\delta\psi\,|_{r=0}=\psi'\delta\psi\,|_{r=0}$, present in Eq, (12), does not appear in Eq. (22) since this term is zero on account of the $\lim_{r\to 0} rV(r)=-Z$ boundary condition.[5]

Let us work out now the first term on the right-hand side of Eq. (22). Considering Eqs. (17) and (18), one finds that

$$\psi'\,|_{r=R_n}\delta\psi\,|_{r=R_n}=\left[\frac{Z}{\epsilon(0)r}\right]\left[-\frac{Z}{\epsilon(0)R_n}\delta R_n\right]\ . \tag{24a}$$

Using Eqs. (16), (18), and (20), one finds that the second term on the right-hand side of Eq. (22) becomes

$$-F\Big|_{r=R_n}\delta R_n=\frac{1}{2}\left[\frac{Z}{\epsilon(0)R_n}\right]^2\delta R_n+\tfrac{2}{5}aR_n^2E_F^{5/2}\delta R_n\ . \tag{24b}$$

With the aid of Eqs. (24a) and (24b), one also finds that Eq. (22) can be brought to the form

$$\delta G=-\frac{1}{2}\left[\frac{Z}{\epsilon(0)R_n}\right]^2\delta R_n+\tfrac{2}{5}aR_n^2E_F^{5/2}\delta R_n\ . \tag{25}$$

Recognizing that $\delta R_n/R_n^2=-\delta(1/R_n)$ and $R_n^2\delta R_n=\frac{1}{3}\delta(R_n^3)$, Eq. (25) can be expressed as

$$\delta G=\frac{1}{2}\left[\frac{Z}{\epsilon(0)}\right]^2\delta\left[\frac{1}{R_n}\right]+\tfrac{2}{15}aE_F^{5/2}\delta(R_n^3)\ . \tag{26}$$

With the result embodied in Eq. (26), the quantity G appearing in Eq. (13) can be taken to be

$$G=\frac{1}{2}\left[\frac{Z}{\epsilon(0)}\right]^2\frac{1}{R_n}+\tfrac{2}{15}aE_F^{5/2}R_n^3\ . \tag{27}$$

With possession of the quantities F and G, the final task consists now in making a choice for the trial function $\psi(r)$ and finding the extremum of the quantity

$$J=\int_0^{R_n}F\,dr+G \tag{28}$$

with respect to the parameters in the trial function. The finding of the extremum of Eq. (28) is, of course, equivalent to the demand expressed by Eq. (13).

Choosing the trial function by

$$\psi(r)=[(1-\lambda)+\lambda e^{-r/r_0}]\times[-Z\sinh q(R_n-r)/\sinh qR_n]\ , \tag{29}$$

where λ and r_0 are variational parameters, it is easy to see that the function in Eq. (29) satisfies the

$$\psi(0)=-Z \tag{30}$$

boundary condition[5] at the origin, and the matching condition at $r=R_n$ that is stated by Eq. (16).

The motivation for the choice of this trial function is the following. For $\lambda=0$ it reduces in form to the solution of the linear case. The prefactor $[(1-\lambda)+\lambda e^{-r/r_0}]$ distorts this form for small r (in the region $0<r\lesssim r_0$); this is the region in which a departure from the form of the linear case is to be expected.[7]

As to matching[5] of $\psi'(r)$ at $r=R_n$, one finds from Eqs. (18) and (29) that

$$[(1-\lambda)+\lambda e^{-R_n/r_o}][Zq/\sinh qR_n]=Z/\epsilon(0)R_n\ . \tag{31}$$

Equation (31) can be solved for λ, yielding the expression

$$\lambda=[1-\sinh qR_n/\epsilon(0)qR_n]\times[1/(1-e^{-R_n/r_0})]\ . \tag{32}$$

Equation (32) gives the parameter λ in terms of the parameters R_n and r_o. These quantities will, from now on, be considered as the variational parameters.

To evaluate the integral in Eq. (28), a new variable defined by

TABLE I. Parameters entering into the spatial dielectric function of diamond. R_n and r_0 are measured in atomic units (Ref. 8).

Z	R_n	λ	r_0
0	2.76	0	
1	2.68	0.079	0.16
2	2.62	0.132	0.17
3	2.56	0.182	0.19
4	2.53	0.205	0.18

$$u = r^{1/2} \tag{33}$$

is introduced. With the new variable u, the singularity in the integrand is eliminated and the integral assumes the form

$$\int_0^{R_n} F\,dr = -\int_0^{\sqrt{R_n}} u(\psi')^2 du - 2a\int_0^{\sqrt{R_n}} E_F^{3/2} u^3 du - \tfrac{4}{5}a\int_0^{\sqrt{R_n}} u^5 (E_F - \psi u^{-2})^{5/2} du \ . \tag{34}$$

The integrals involved in Eq. (34) have all been evaluated by numerical integration.

The parameter values R_n and r_0, at which J in Eq. (28) assumes its extremum for point charges $Z = +1, +2, +3, +4$ in pure diamond, silicon, and germanium, are given in Tables I–III. These tables also list the parameter values for λ.

Finally, the spatial dielectric function $\bar{\epsilon}_n(r)$, as defined by Eq. (1), is

$$\bar{\epsilon}_n(r) = -\frac{Z}{rV(r)} \ , \tag{35}$$

which, by making use of Eq. (14), can be written as

$$\bar{\epsilon}_n(r) = -\frac{Z}{\psi(r) + rA} \ . \tag{36}$$

Using Eqs. (6) and (31), Eq. (36) can be brought to the form

TABLE II. Parameters entering into the spatial dielectric function of silicon. R_n and r_0 are measured in atomic units (Ref. 8).

Z	R_n	λ	r_0
0	4.28	0	
1	4.12	0.141	0.24
2	4.00	0.225	0.26
3	3.91	0.282	0.27
4	3.85	0.317	0.26

TABLE III. Parameters entering into the spatial dielectric function of germanium. R_n and r_0 are measured in atomic units (Ref. 8).

Z	R_n	λ	r_0
0	4.54	0	
1	4.40	0.125	0.21
2	4.27	0.220	0.26
3	4.20	0.267	0.25
4	4.14	0.304	0.25

$$\bar{\epsilon}_n(r) = \left[[(1-\lambda) + \lambda e^{-r/r_0}] \left[\frac{\sinh q(R_n - r)}{\sinh q R_n} \right] + \frac{r}{\epsilon(0) R_n} \right]^{-1} , \tag{37}$$

which is the central result of this paper. The spatial dielectric function $\epsilon_n(r)$ for charges $Z = +1$, $+4$ in silicon, is illustrated in Fig. 1. The figure also shows the $Z = 0$ result of the linearized theory.

III. DISCUSSION

Inspection of Fig. 1 shows that the $Z = +4$ curve deviates more significantly from the $Z = 0$ curve than does the $Z = +1$ curve. This has already been established by Cornolti and Resta.[5] The $Z = +2, +3$ curves are not shown in Fig. 1, to avoid overcrowding the illustration. They both lie in the area bordered by the $Z = +1$ and $Z = +4$ curves, with the $Z = +2$ curve closer to the $Z = 0$ curve than the $Z = +3$ curve.

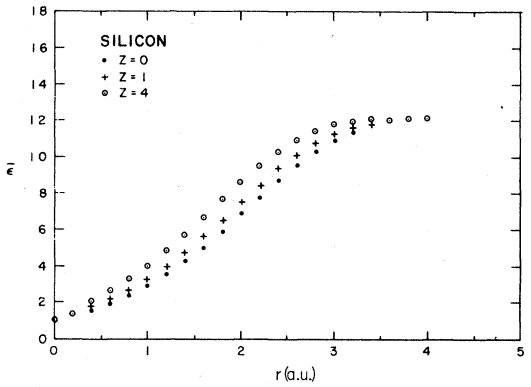

Fig. 1. The spatial dielectric function of silicon [Eq. (37)] versus the distance (in a.u.) from the charge.

Finally, it is mentioned that the corresponding $\bar{\epsilon}_n(r)$ versus r curves in diamond and germanium are quite similar to those shown in Fig. 1. For the purpose of saving space, they are not given here.

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[1]For a list of applications, see Ref. 2

[2]R. Resta, Phys. Rev. B 16, 2717 (1977).

[3]Following the terminology of Ref. 5, we shall refer to the potential energy as the potential.

[4]In the present work, the q value used for Ge is not that given in Ref. 2, but that (1.12) which is inferred from Ref. 5.

[5]F. Cornolti and R. Resta, Phys. Rev. B 17, 3239 (1978).

[6]Since linearization is exact when $Z \to 0$, we shall refer to $\bar{\epsilon}_l(r)$ as the $Z=0$ case.

[7]P. Csavinszky, Phys. Rev. B 21, 632 (1980).

[8]$\hbar=1$, $e^2=1$, $m_e=1$, unit of length is a_B, the first Bohr radius in the H atom.

[9]R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1966), Vol. I, p. 260.

[10]It is important to note that although R_n appeared explicitly in the original differential equation (1) [via $A=\psi(R_n)$], the change of dependent variable (14) has rendered the quantity F to be independent (explicitly) of R_n. If F did depend explicitly on R_n then an additional term, $\int_0^{R_n} (\partial F/\partial R_n) dr\, \delta R_n$, would appear in Eq. (10).