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

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In the present paper we formulate a variational principle for obtaining approximate analytical solutions of a nonlinear differential equation established by Cornolti and Resta for the potentials of *negative* point charges embedded in pure diamond, silicon,and germanium. We consider the case of charges $Z=-1$, -2, -3, and -4 (in atomic units) in these semiconductors, while Cornolti and Resta considered the cases of $Z=-1$ and -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 graphical form.

I. INTRODUCTION

Recently Resta[1] has formulated a nonlinear Thomas-Fermi (TF) approach for obtaining the potentials of positive and negative point charges embedded in pure semiconductors. In another work, Cornolti and Resta[2] have numerically solved Resta's nonlinear TF equation for the potential of positive and negative point charges embedded in pure diamond, silicon, and germanium. These authors have presented graphical results for $\bar{\epsilon}_n(r)$, the spatial dielectric function associated with the nonlinear theory, for point charges $Z=\pm 1,\pm 4$ (in atomic units).

Very recently Csavinszky and Brownstein[3] have obtained $\bar{\epsilon}_n(r)$ analytically for point charges $Z=+1,+2,+3,+4$ in pure diamond, silicon, and germanium. The approximate analytical solution for $\bar{\epsilon}_n(r)$ was made feasible by an equivalent variational principle to the nonlinear TF equation.[1,2]

In the present paper we have extended our variational approach to the potentials of point charges $Z=-1,-2,-3,-4$ in pure diamond, silicon, and germanium. In what follows we present our theory in a terse manner since the necessary mathematical framework is detailed in our previous work[3] (hereafter referred to as I). As in I, all quantities are written using atomic units.[4]

II. THEORY

The nonlinear TF equation[1,2] solved by Cornolti and Resta[2] is

$$\nabla^2 V(r)=\begin{cases}0, & R_n\le r<\infty\\ a\{E_F^{3/2}-[E_F+A-V(r)]^{3/2}\}, & R_c\le r<R_n\\ aE_F^{3/2}, & 0<r\le R_c\end{cases} \tag{1}$$

where $a=2^{7/2}/3\pi$ and $A=V(R_n)$. In Eq. (1), V is the potential of the negative point charge embedded into the pure semiconductor, R_n is a screening radius,[2,3] R_c is the radius of the Coulomb hole,[2] defined by

$$E_F+A-V(R_c)=0\ , \tag{2}$$

and E_F denotes the valence Fermi energy which is related to the valence Fermi momentum by $E_F=k_F^2/2$.

Introducing the function

$$\psi(r)=r[V(r)-A]\ , \tag{3}$$

Eq. (1) is transformed into

$$\psi''=\begin{cases}0, & R_n\le r<\infty\\ a[rE_F^{3/2}-r(E_F-\psi/r)^{3/2}], & R_c\le r\le R_n\\ arE_F^{3/2}, & 0<r\le R_c\ .\end{cases} \tag{4}$$

This equation differs from that for a positive point charge[3] by the presence of the last line. (For a positive point charge, the regions of interest are $R_n\le r<\infty$ and $0<r\le R_n$.)

For $r\ge R_n$, the solution is[2,3]

$$V=-\frac{Z}{\epsilon(0)r}\ , \tag{5}$$

where $\epsilon(0)$ is the static dielectric constant of the semiconductor. We note here that with the aid of Eq. (3) the definition of R_c becomes

$$\psi(R_c)=R_cE_F\ . \tag{6}$$

It is easy to show that $\psi<rE_F$ for $r>R_c$, and $\psi>rE_F$ for $r<R_c$. Our goal is to solve Eq. (4), in an approximate analytical form, by an equivalent variational principle. As shown in I, the variational principle can be established by working out the (first) variation of the integral

$$I=\int_0^{R_n}F(\psi,\psi',r)dr\ . \tag{7}$$

We note here that, in the terminology of Courant and Hilbert,[5] our variational problem is of "variable domain" type since not only the function $\psi(r)$ but also the upper limit R_n is a variable. As shown in I, the variational principle can be stated by finding the extremum of

$$J=\int_0^{R_n}F\,dr+G\ , \tag{8}$$

where, with the F chosen below,

$$G=\frac{1}{2}\left[\frac{Z}{\epsilon(0)}\right]^2\frac{1}{R_n}+\frac{2}{15}aE_F^{5/2}R_n^3\ . \tag{9}$$

The quantity F in Eq. (8) has to be chosen in such a manner that upon its substitution into the Euler-Lagrange equation

$$-\frac{d}{dr}\frac{\partial F}{\partial\psi'}+\frac{\partial F}{\partial\psi}=0\ , \tag{10}$$

one recovers Eq. (4) over $0<r\le R_n$. Let us choose F by

$$F=-\tfrac{1}{2}(\psi')^2 -a[rE_F^{3/2}\psi+S(rE_F-\psi)\tfrac{2}{5}r^2(E_F-\psi/r)^{5/2}]\ , \tag{11}$$

where S is the unit step function, i.e.,

$$S(z)=\begin{cases}0, & z<0\\ 1, & z\ge 0\ .\end{cases} \tag{12}$$

Substitution of Eq. (11) into Eq. (10) leads to

$$\psi''=a\left[rE_F^{3/2}-S(rE_F-\psi)r\left[E_F-\frac{\psi}{r}\right]^{3/2}\right] -aS'(rE_F-\psi)\tfrac{2}{5}r^2\left[E_F-\frac{\psi}{r}\right]^{5/2}\ , \tag{13}$$

where S', i.e., the derivative of S with respect to its argument, is $\delta(rE_F-\psi)$. This delta function is, however, multiplied by $(E_F-\psi/r)^{5/2}$ which equals zero for $rE_F=\psi$. For this reason, the term involving S' in Eq. (13) vanishes. In view of this, Eq. (13) becomes

$$\psi''=\begin{cases}a[rE_F^{3/2}-r(E_F-\frac{\psi}{r})^{3/2}], & R_c\le r\le R_n\\ arE_F^{3/2}, & 0<r\le R_c\end{cases} \tag{14}$$

which is correct for $0<r\le R_n$.

The final task consists now in making a choice for the trial function $\psi(r)$ and finding the extremum of J in Eq. (8) with respect to the parameters in the trial function. As in I, the trial function is chosen by

$$\psi(r)=[(1-\lambda)+\lambda e^{-r/r_0}] \times[-Z\sinh q(R_n-r)/\sinh qR_n], \qquad 0<r\le R_n \tag{15}$$

where λ and r_0 are variational parameters, and the quantity q is a constant defined[2,3] by $q=(4k_F/\pi)^{1/2}$. It is easy to see that the function in Eq. (15) satisfies the $\psi(0)=-Z$ boundary condition[2] at the origin and the matching condition[2] for $\psi(R_n)$. It also satisfies all matching conditions[2] (on ψ and ψ') at $r=R_c$.

The motivation for the choice of this trial function is the following. For $\lambda=0$, it reduces in form to the solution[1] of the linearized TF equation. Ap-

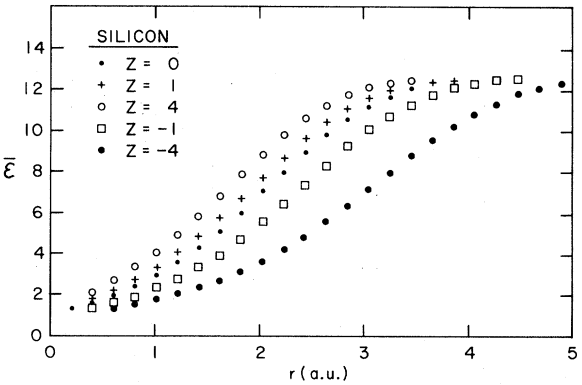

FIG. 1. The spatial dielectric function of silicon [Eq. (18)] versus the distance (in a.u.) from the charge.

TABLE I. Parameters entering into the spatial dielectric function of diamond for which $\epsilon(0)$ is 5.7 and q is 1.36 a.u.

Z	R_n (a.u.)	λ	r_0 (a.u.)
0	2.76	0	
−1	2.97	−0.233	0.47
−2	3.18	−0.544	0.85
−3	3.30	−0.769	1.04
−4	3.43	−1.077	1.34

TABLE III. Parameters entering into the spatial dielectric function of germanium for which $\epsilon(0)$ is 16 and q is 1.12 a.u. (Ref. 8).

Z	R_n (a.u.)	λ	r_0 (a.u.)
0	4.54	0	
−1	4.97	−0.469	0.92
−2	5.27	−0.965	1.50
−3	5.61	−1.895	2.68
−4	5.95	−3.953	5.28

plying the matching condition for $\psi'(r)$ at $r=R_n$, one finds[3] that

$$\lambda=[1-\sinh qR_n/\epsilon(0)qR_n][1/(1-e^{-R_n/r_0})] , \tag{16}$$

which gives the parameter λ in terms of the parameters R_n and r_0. These quantities will, from now on, be considered as the variational parameters.

The evaluation of the integral in Eq. (8) is discussed in I. It is also shown in I that the spatial dielectric function $\bar{\epsilon}_n(r)$, defined by

$$\bar{\epsilon}_n(r)=-\frac{Z}{rV(r)} \tag{17}$$

can be expressed by

$$\bar{\epsilon}_n(r)=\left[[(1-\lambda)+\lambda e^{-r/r_0}][\sinh q(R_n-r)/\sinh qR_n]+\frac{r}{\epsilon(0)R_n}\right]^{-1} . \tag{18}$$

Equation (18) is the central result of this paper.

The spatial dielectric function $\bar{\epsilon}_n(r)$ for charges $Z=-1$, -4 in silicon, is illustrated in Fig. 1. The figure also shows the $Z=0$ result[1] of the linearized theory, and, for comparison, the $Z=+1$, $+4$ results of I. In Tables I, II, and III we list the parameter values R_c, R_n, λ, and r_0 for changes $Z=-1$, -2, -3, -4, in pure diamond, silicon, and germanium. The values of $\epsilon(0)$ and q, entering into Eq. (18), are listed in the respective table captions.

TABLE II. Parameters entering into the spatial dielectric function of silicon for which $\epsilon(0)$ is 11.94 and q is 1.10 a.u.

Z	R_n (a.u.)	λ	r_0 (a.u.)
0	4.28	0	
−1	4.75	−0.492	0.96
−2	5.07	−1.026	1.60
−3	5.45	−2.179	3.11
−4	5.78	−4.628	6.23

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.[2] 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.

Inspection of Fig. 1 also shows that the $Z=-1$ curve lies further from the $Z=0$ curve[6] than does the $Z=+1$ curve. The same situation prevails also with respect to the $Z=-4$ and $Z=+4$ curves. This is in accord with the finding of Cornolti and Resta.[2] The numerical solution[7] of Eq. (1) agrees remarkably well with the analytical solution. On the scale of the figure the former is almost indistinguishable from the latter. 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.

[1]R. Resta, Phys. Rev. B 16, 2717 (1977).
[2]F. Cornolti and R. Resta, Phys. Rev. B 17, 3239 (1978).
[3]P. Csavinszky and K. R. Brownstein, Phys. Rev. B (in press).
[4]$\hbar=1$, $e^2=1$, $m_e=1$, unit of length is a_B, the first Bohr radius in the H atom.
[5]R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1966), Vol. I, p. 260.
[6]Since linearization is exact when $Z\rightarrow 0$, we shall refer to $\bar{\epsilon}_l(r)$, the spatial dielectric function of the linearized theory, as the $Z=0$ case.
[7]We have also solved numerically both the linearized and the nonlinear TF equations.
[8]In the present work the q value used for Ge is not that given in Ref. 1, but that (1.12) which is inferred from Ref. 2.