Asymptotic corrections to the potential of impurity ions in semiconductors with spatially variable dielectric constants

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In a recent paper, the problem of the screening of a (point) donor ion in Si and Ge has been reexamined by introducing into the theory the spatial dielectric functions of Azuma and Shindo and Okuro and Azuma, respectively. Poisson's equation, with the neglect of a small term, has been solved approximately by making use of a variational principle. The result was an impurity-ion potential that consists of a linear combination of two exponentially screened Coulomb potentials (with two different screening lengths) which is scaled by the static dielectric constant of the medium. The present paper shows that, at distances larger than Dingle's screening length R_0, the term neglected in Poisson's equation would add to this impurity-ion potential two types of correction. One type consists of terms which are proportional to Dingle's potential, but with proportionality constants so small that the correction terms are rendered utterly negligible. The other type consists of terms each one of which is proportional to functions of the form $(1/r^m)\exp(-q_i r)$, where $m = 2, 3, 4, \ldots$, and the parameters q_i are related to the constants appearing in the spatial dielectric functions of Si and Ge. The finding that the correction terms to the impurity-ion potential fall off faster than $1/r$ does, in the author's opinion, establish the asymptotic validity of the previous variational theory.

Poisson's equation, for the potential $\phi(r)$ of a (point) donor ion, in a medium characterized by a spatial dielectric function $\kappa(r)$, has the form[1]

$$\nabla^2\phi(r) + \frac{4\pi\rho(r)}{\kappa(r)} = -\frac{1}{\kappa(r)}\frac{d\kappa(r)}{dr}\frac{d\varphi(r)}{dr} , \quad (1)$$

where $\rho(r)$, the density of the screening charge, is composed of mobile electrons.

The spatial dielectric function, for Si (Ref. 2) and Ge (Ref. 3), has the form

$$1/\kappa(r) = 1/\kappa_0 + e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r} , \quad (2)$$

where κ_0 is the static dielectric constant of the respective medium, and the quantities α, β, γ, A, and B are constants which are given in Table I.

Making use of a previous investigation[4] of the right-hand side of Eq. (1), and introducing the function $\psi(r)$ by

$$\psi(r) = r\varphi(r) , \quad (3)$$

one can cast Eq. (1) into the simpler form

$$\psi''(r) - R_0^{-2}\psi(r) - \kappa_0 R_0^{-2}\psi(r)[e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r}] = \left(\frac{d}{dr}[\ln(1+\kappa_0 f)]\right)\left(\psi'(r) - \frac{\psi(r)}{r}\right) , \quad (4)$$

where R_0 is a constant, and the quantity f is defined by

$$f = e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r} . \quad (5)$$

Replacing $\ln(1+\kappa_0 f)$ by $\kappa_0 f$, the first term of its expansion,[5] one finds that Eq. (4) becomes

$$\psi''(r) - R_0^{-2}\psi(r) - \kappa_0 R_0^{-2}\psi(r)[e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r}] = -\kappa_0[\alpha e^{-\alpha r} - A\beta e^{-\beta r} - B\gamma e^{-\gamma r}] \times [\psi'(r) - \psi(r)/r] . \quad (6)$$

Let us digress now for a minute and consider the inhomogeneous differential equation

$$y''(x) + P(x)y'(x) + Q(x)y(x) = S(x) . \quad (7)$$

Assuming that the solutions of the corresponding homogeneous differential equation are known, and are denoted by $u_1(x)$ and $u_2(x)$, a particular solution of Eq. (8) is obtained from[6]

$$y_p(x) = \int_\lambda^x \frac{u_1(t)u_2(x) - u_2(t)u_1(x)}{u_1(t)u_2'(t) - u_2(t)u_1'(t)} S(t)\, dt , \quad (8)$$

where λ is a constant, as yet not specified.

Considering the right-hand side of Eq. (6) as the function $S(t)$, Eq. (8) permits one to derive an ap-

TABLE I. Parameters in the spatial dielectric function. (It appears that there are two misprints in Ref. 2. The parameter β is given as $9.129a_B^{-1}$, while the parameter γ is given as $0.0302a_B^{-1}$. Figure 1 of Ref. 2 can, however, be reproduced only with the values of $\beta = 0.9129a_B^{-1}$ and $\gamma = 0.302a_B^{-1}$, respectively.)

Semiconductor	A	B	α (a_B^{-1})	β (a_B^{-1})	γ (a_B^{-1})
Ge	0.0544	0.0080	0.9668	0.3757	0.7460
Si	0.0726	0.0107	0.663	0.9129	0.302

proximate value for $\psi_p(r)$ since the two approximate solutions of the corresponding homogeneous equation, obtained[1] from a variational principle, are known to be[7]

$$\psi_1(r) = (e_0/\kappa_0)[Ce^{-r/R_1} + (1-C)e^{-r/R_2}] \tag{9}$$

and

$$\psi_2(r) = (e_0/\kappa_0)[Ce^{+r/R_1} + (1-C)e^{+r/R_2}] \ . \tag{10}$$

In Eqs. (9) and (10), e_0 is the magnitude of the electron charge, C is a constant,[1] and the quantities R_1 and R_2 are screening lengths, defined[1] by

$$R_1 = R_0/(1-n) \tag{11}$$

and

$$R_2 = R_0/(1+n) \ , \tag{12}$$

where n is a constant,[1] and R_0 denotes a screening length introduced by Dingle.[8]

A modest effort will suffice to convince one that Eq. (8) cannot be evaluated in a closed form with the functions displayed in Eqs. (9) and (10). For this reason, as an approximation, the solutions[9] of Eq. (1) with $\kappa(r) = \kappa_0$ will be used for the evaluation of Eq. (8). These solutions are given by

$$\psi_{01}(r) = \tfrac{1}{2}(e_0/\kappa_0)e^{-r/R_0} \tag{13}$$

and

$$\psi_{02}(r) = \tfrac{1}{2}(e_0/\kappa_0)e^{+r/R_0} \ . \tag{14}$$

The boundary conditions, both in Dingle's theory[8] and in its subsequent generalization,[1] are

$$\psi_0(0) = e_0/\kappa_0 \tag{15}$$

and

$$\psi_0(\infty) = 0 \ , \tag{16}$$

where $\psi_0(r)$, the general solution of Eq. (1) with $\kappa(r) = \kappa_0$, is the sum of the functions displayed in Eqs. (13) and (14). A glance at these equations shows that ψ_0 satisfies Eq. (15) but does not satisfy Eq. (16). Use of Eqs. (13) and (14) for the evaluation of Eq. (8) does not, however, violate any principle since it is the solution of the complete equation (which includes ψ_p) on which the boundary conditions must be imposed.

With these considerations, Eq. (8) can be written as

$$\psi_p(r) = -\frac{\kappa_0 R_0}{2}\int_{r_0}^{r} (e^{-t/R_0}e^{+r/R_0} - e^{+t/R_0}e^{-r/R_0}) \times (\alpha e^{-\alpha t} - A\beta e^{-\beta t} - B\gamma e^{-\gamma t}) \times [\psi_0'(t) - \psi_0(t)/t]\, dt \ , \tag{17}$$

where the notation $\lambda = r_0$, with r_0 as yet unspecified, has been introduced.

In what follows, Eq. (17) will be written as

$$\psi_p(r) = \psi_p^{\rm I}(r) + \psi_p^{\rm II}(r) \ , \tag{18}$$

where $\psi_p^{\rm I}(r)$ goes with the first term in the square brackets, while $\psi_p^{\rm II}(r)$ goes with the second term (including the minus sign).

Evaluating the integrals involved in $\psi_p^{\rm I}$, and dropping terms multiplied by e^{+r/R_0} times a constant [since they are incompatible with the boundary condition in Eq. (16)], one obtains, upon consideration of Eq. (3),

$$\varphi_p^{\rm I}(r) = -\frac{e_0}{4}\left[\frac{e^{-r/R_0}}{r}\left(e^{-\alpha r_0} - \frac{\alpha}{\alpha - 2R_0^{-1}}e^{-(\alpha - 2R_0^{-1})r_0}\right) + \frac{e^{-(\alpha + R_0^{-1})r}}{r}\left(\frac{\alpha}{\alpha + 2R_0^{-1}} - 1\right) + \frac{e^{-(\alpha - R_0^{-1})r}}{r}\left(\frac{\alpha}{\alpha - 2R_0^{-1}} - 1\right)\right]$$
$$+\text{similar terms involving } \beta \text{ and } \gamma. \tag{19}$$

Considering the definition of the exponential integral,[10]

$$-E_i(-\xi) = \int_\xi^\infty \frac{e^{-z}}{z}\, dz \ , \tag{20}$$

and using the symbolism $\int_{r_0}^{r} = \int_{r_0}^{\infty} - \int_{r}^{\infty}$, one finds, upon consideration of Eq. (3) and upon dropping terms in e^{+r/R_0} times a constant, that

$$\varphi_p^{\rm II}(r)\Big/\left(-\frac{e_0 R_0}{4r}\right) = -\alpha e^{-r/R_0}\{[-Ei(-\alpha r)] + [-E_i(-\delta_\alpha r)]\} + \alpha e^{-r/R_0}\{[-Ei(-\alpha r_0)] + [-Ei(-\delta_\alpha r_0]\} + \alpha e^{+r/R_0}\{[-Ei(-\alpha r)] + [-Ei(-\bar{\delta}_\alpha r)]\}$$
$$+\text{similar terms involving } \beta \text{ and } \gamma, \tag{21}$$

where

$$\delta_j = j - 2R_0^{-1} \tag{22}$$

and

$$\bar{\delta}_j = j + 2R_0^{-1} \tag{23}$$

with $j = \alpha, \beta, \gamma$.

To proceed, use is made of the relation[11]

$$e^{\xi}[-Ei(-\xi)] = \frac{0!}{\xi} - \frac{1!}{\xi^2} + \frac{2!}{\xi^3} - \frac{3!}{\xi^4} + \cdots \ , \tag{24}$$

which permits one to rewrite Eq. (21). The result, involving only the first term on the right-hand side of Eq. (24), is given by

$$\phi_p^{\mathrm{II}}(r) = -\frac{e_0}{4}\left[\frac{e^{-r/R_0}}{r}\left(\frac{R_0}{r_0}\, e^{-\alpha r_0} + \frac{\alpha}{\alpha - 2R_0^{-1}}\,\frac{R_0}{r_0}\, e^{-(\alpha - 2R_0^{-1})r_0}\right) + \frac{e^{-(\alpha + R_0^{-1})r}}{r^2}\left(\frac{\alpha}{\alpha + 2R_0^{-1}} - 1\right)R_0 - \frac{e^{-(\alpha - R_0^{-1})r}}{r^2}\left(\frac{\alpha}{\alpha - 2R_0^{-1}} - 1\right)R_0\right] + \text{similar terms in } \beta \text{ and } \gamma . \quad (25)$$

At this stage, a choice for r_0 has to be made. In principle, the smallest value of r_0, permitted in the present treatment, could be that value of r at which the expansion of $\ln(1+\kappa_0 f)$, in Eq. (4), is permissible. Knowing that this is the case when $-1<\kappa_0 f<+1$, one might say that r_0 could be determined from $\kappa_0 f = 1$. This r value, with the constants displayed in Table I, turns out to be $r_0 = 6.0 a_B$ for Si, and $r_0 = 3.8 a_B$ for Ge, where a_B stands for the Bohr radius. The above choice for r_0, however, would be an extremely crude one since Eq. (6) is based on the retention of only the first term of the infinite series for $\ln(1+\kappa_0 f)$ which is a good approximation only when $\kappa_0 f \ll 1$. Instead of proceeding along these lines, one might just as well inquire about the contribution to the variationally obtained impurity-ion potential[1] that results from the right-hand side of Eq. (1) at $r > R_0$. This appears to be a reasonable question since the screening length R_0 is a quantity that characterizes the "range" of the exponentially screened Coulomb potential. For this reason, the choice $r_0 = R_0$ is made and then the sum of Eqs. (19) and (25) is found to be

$$\begin{aligned}\varphi_p(r) = &-\frac{e_0}{2}\, e^{-\alpha R_0}\,\frac{e^{-r/R_0}}{r} - \frac{e_0}{4}\left[\frac{\alpha}{\alpha + 2R_0^{-1}} - 1\right]\frac{e^{-(\alpha + R_0^{-1})r}}{r} - \frac{e_0}{4}\left[\frac{\alpha}{\alpha - 2R_0^{-1}} - 1\right]\frac{e^{-(\alpha - R_0^{-1})r}}{r} \\ &- \frac{e_0 R_0}{4}\left[\frac{\alpha}{\alpha + 2R_0^{-1}} - 1\right]\frac{e^{-(\alpha + R_0^{-1})r}}{r^2} + \frac{e_0 R_0}{4}\left[\frac{\alpha}{\alpha - 2R_0^{-1}} - 1\right]\frac{e^{-(\alpha - R_0^{-1})r}}{r^2} \\ &+ \text{similar terms in } \beta \text{ and } \gamma . \end{aligned} \quad (26)$$

For all physically significant cases $R_0 \gg 1$, so that $2R_0^{-1}$ is very small compared to α. For this reason, a binomial expansion of the first term in each of the square brackets can be carried out. Retaining terms up to and including $(2R_0^{-1})/\alpha$, one finds that Eq. (26) reduces to

$$\begin{aligned}\phi_p(r) = &-\frac{e^{-\alpha R_0}}{2}\,\frac{e_0 e^{-r/R_0}}{r} + \frac{1}{2\alpha R_0}\,\frac{e_0 e^{-(\alpha + R_0^{-1})r}}{r} - \frac{1}{2\alpha R_0}\,\frac{e_0 e^{-(\alpha - R_0^{-1})r}}{r} + \frac{1}{2\alpha}\,\frac{e_0 e^{-(\alpha + R_0^{-1})r}}{r^2} \\ &+ \frac{1}{2\alpha}\,\frac{e_0 e^{-(\alpha - R_0^{-1})r}}{r^2} + \text{similar terms in } \beta \text{ and } \gamma . \end{aligned} \quad (27)$$

Upon the further neglect of R_0^{-1} in the exponents, Eq. (27) becomes

$$\phi_p(r) = -\frac{e^{-\alpha R_0}}{2}\,\frac{e_0 e^{-r/R_0}}{r} + \frac{1}{\alpha}\,\frac{e_0 e^{-\alpha r}}{r^2} + \text{similar terms in } \beta \text{ and } \gamma . \quad (28)$$

The first term on the right-hand side of Eq. (28) is utterly negligible. The reason is, that the parameter α is of the order unity, while the parameter R_0 is, even in a degenerate semiconductor, more than an order of magnitude larger than α.

The factor $e^{-\alpha r}/r^2$ in the second term on the right-hand side of Eq. (28) is also negligible when compared to the factor $e^{-r/R_0}/r$, appearing in the Dingle potential.

In summary, it has been shown that, with a specific analytical choice for the spatial dielectric functions of Si and Ge, the contribution of a neglected term (in Poisson's equation) to the donor-ion potential (of Ref. 1) is of an asymptotic nature when compared with

$$[e_0/(\kappa_0 r)][C e^{-r/R_1} + (1 - C) e^{-r/R_2}] .$$

[1]P. Csavinszky, Phys. Rev. B 14, 1649 (1976). There are some misprints in this paper. In Eq. (7), the factor under the square root should read $(2\pi k_B T)^{1/2}$. In Eq. (18a), the sign following ϕ'' should be plus. In Eq. (32), the denominator should read ∂b. In Eq. (39), the minus sign should precede 1. The year of the first reference should be (1946).
[2]M. Azuma and K. Shindo, J. Phys. Soc. Jpn. 19, 424 (1964).
[3]S. Okuro and M. Azuma, J. Phys. Soc. Jpn. 20, 1099 (1964).

[4]P. Csavinszky, Int. J. Quant. Chem. Symp. 10, 305 (1976). In this paper, the right-hand side of Eq. (18) should be multiplied by r.

[5]Using the parameters for Si (Ref. 2) and Ge (Ref. 3), one can easily show that this procedure is completely justified for $r \gtrsim R_0$, the region of interest here.

[6]L. R. Ford, *Differential Equations* (McGraw-Hill, New York, 1955), 2nd ed., p. 72ff.

[7]In Ref. 1, only Eq. (9) has been discussed. It is, however, obvious that, to the same degree of approximation, Eq. (10) is also a solution of the homogeneous equation of Eq. (6), albeit one that does not satisfy the boundary condition in Eq. (16).

[8]R. B. Dingle, Philos. Mag. 46, 831 (1955).

[9]See Sec. II of Ref. 1.

[10]G. Arfken, *Mathematical Methods for Physicists* (Academic, New York, 1970), 2nd ed., p. 290ff.

[11]See Ref. 10, p. 291.