Comments

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Comment on: "Electron mobilities based on an exact numerical analysis of the dielectric-function-dependent linearized Poisson's equation for the potential of impurity ions in semiconductors"

P. Csavinszky and R. A. Morrow
Department of Physics, University of Maine, Orono, Maine 04469
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We believe that an assumption made in this paper, namely, forcing the potential to exhibit a prescribed behavior at a certain distance from a point ion, is not tenable. We present below results of our numerical and variational calculations made without the above assumption.

In a recent paper, Scarfone and Richardson[1] (SR) numerically solve the linearized version of a generalized Poisson equation that has been established by Csavinszky[2] for the potential $\phi(r)$ of a point donor ion in a semiconductor. The nonlinear differential equation is of the form[3]

$$\phi'' + \left(\frac{2}{r} + \frac{\kappa'}{\kappa}\right)\phi' + \frac{4\pi\rho}{\kappa} = 0 , \tag{1}$$

where $\kappa(r)$ has been dubbed[2] the "spatially-variable dielectric constant," and $\rho(r)$ is the electronic screening charge density. Upon linearization we obtain[4]

$$\rho = -\frac{\kappa_0 R_0^{-2}}{4\pi}\phi , \tag{2}$$

which permits us to rewrite Eq. (1) as

$$\phi'' + \left(\frac{2}{r} + \frac{\kappa'}{\kappa}\right)\phi' - \frac{\kappa_0 R_0^{-2}}{\kappa}\phi = 0 , \tag{3}$$

where R_0 is a screening length introduced by Dingle,[5] and κ_0 is the static dielectric constant of the semiconductor. This is the basic differential equation we are going to discuss.[6]

SR have numerically solved Eq. (3) under the assumption that the donor-ion potential $\phi(r)$ at a distance of $r = 25\ a_B$ (a_B stands for the Bohr radius) becomes equal to the Dingle[5] potential

$$\phi_0 = \frac{e_0}{\kappa_0 r} e^{-r/R_0} , \tag{4}$$

where e_0 is the magnitude of the electronic charge. Having solved Eq. (3), subject to the boundary condition given in Eq. (4), SR then obtained a fit of the numerical potential (for a given R_0) to the analytical form of

$$\phi_2 = \phi_0[1 + (\kappa_0 - 1)e^{-tr}] , \tag{5}$$

where t is the fitting parameter and r is measured in units of a_B.

We believe that the above assumption made by SR is not tenable and that it affects the extensive t versus R_0 tables given by them for Si, Ge, and GaAs. Our reason for this belief is as follows. The second-order linear differential equation given in Eq. (3) must be solved subject to two boundary conditions. These boundary conditions specify the behavior of the potential near the origin, $\phi(r \to 0) = e_0/r$, and at infinity, $\phi(r \to \infty) = 0$. The correct solution is then uniquely determined at all intermediate values of r. It does not follow that the solution at any particular value of r, say r_0, is given by $\phi_0(r_0)$ of Eq. (4). By forcing this requirement at $r_0 = 25$ a.u., SR have necessarily obtained a solution that violates one of the boundary conditions.

We have solved Eq. (3) subject to the proper boundary conditions for Si [with a $\kappa(r)$ we shall discuss momentarily] both by numerical means[7] and by an equivalent variational principle proposed by Csavinszky and Morrow.[8] We find that a variational trial potential of the form

$$\phi_v = \phi_0[q + (\kappa_0 - q)e^{-pr}] , \tag{6}$$

where q and p are variational parameters, and r is again measured in units of a_B, is in very good agreement with our numerical potential. This is

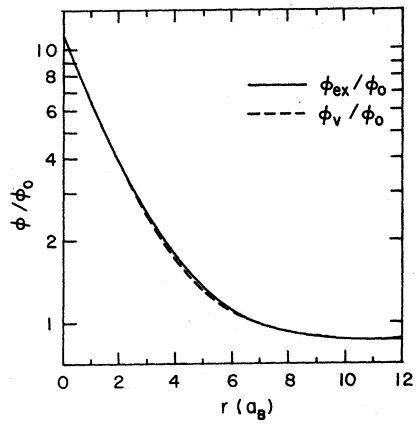

FIG. 1. Comparison of the approximate variational potential ϕ_v (normalized to the Dingle potential ϕ_0) with the exact numerical potential ϕ_{ex} (normalized to the Dingle potential ϕ_0). The potentials have been obtained (Ref. 14) for a point donor ion in uncompensated n-type Si using a screening length of $R_0 = 11.3\, a_B$.

illustrated for[9] $R_0 = 11.3\, a_B$ in Fig. 1. We also find that the variational parameter p is a sensitive function of R_0. This is illustrated in Fig. 2. A sensitivity on R_0 is also exhibited by the variational parameter q, which is illustrated in Fig. 3. Our finding concerning the exponential parameter p is very different from that of SR, who find that the exponential parameter t is almost a constant over a wide range of R_0 values.

Let us return now to the assumption made by SR. At $r = 25\, a_B$, the exponential factor in the square brackets in Eq. (6) is (using Fig. 2 to obtain the required p value) $e^{-(0.64)(25)} = e^{-16} = 0.11 \times 10^{-6}$. This number, even when multiplied by $(\kappa_0 - q)$, is completely negligible compared to $q = 0.85$ (obtained from Fig. 3). Consequently, for $r \geq R_0$, Eq. (6) can be written as

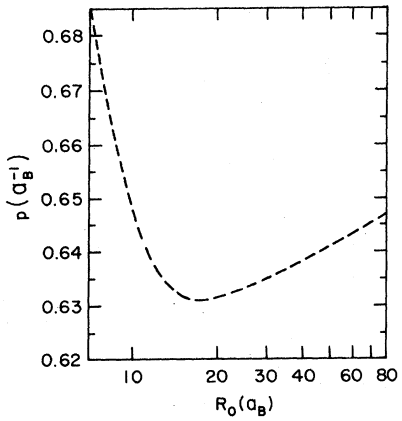

FIG. 2. Dependence (Ref. 14) of the variational parameter p on the screening length R_0 in n-type uncompensated Si.

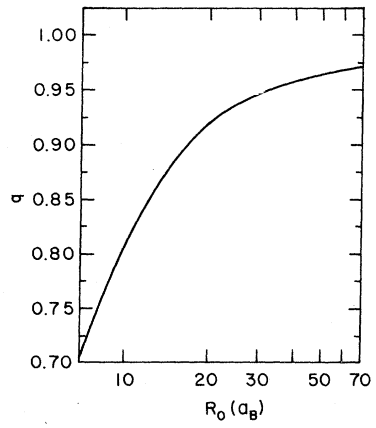

FIG. 3. Dependence (Ref. 14) of the variational parameter q on the screening length R_0 in n-type uncompensated Si.

$$\phi_v/\phi_0 = q < 1\,, \tag{7}$$

in conflict with SR. One other comment concerning Eq. (3) must be made.

In our calculations we have not identified the spatial dielectric function $\epsilon(r)$ with the spatially-variable dielectric constant $\kappa(r)$, as has been done by SR. Our reasons for this distinction, as has been put forward by Morrow and Csavinszky,[10] are stated below.

The spatial dielectric function $\epsilon(r)$ describes the response of an undoped semiconductor to a perturbing point charge. This quantity, for a point donor ion placed into the undoped semiconductor, is defined[11] by

$$\varphi = \frac{e_0}{r\epsilon(r)}\,. \tag{8}$$

On the basis of Eq. (8), $\epsilon(r)$ can be interpreted as the unshielded potential (e_0/r) divided by the shielded potential (φ).

On the other hand, the spatially-variable dielectric constant $\kappa(r)$ enters into the theory[2] of the potential of a point donor ion placed into a doped semiconductor. This quantity may be defined by

$$\vec{E} = \frac{e_0}{\kappa(r)}\,\frac{\vec{r}}{r^3}\,, \tag{9}$$

from which $\kappa(r)$ may be interpreted as the unshielded electric field $(e_0\vec{r}/r^3)$ divided by the shielded electric field $(\vec{E})$.

Using $\vec{E}(r) = -\vec{\nabla}\phi(r)$, it follows from Eqs. (8) and (9) that[12]

$$\frac{1}{\kappa(r)} = \frac{1}{\epsilon(r)} - r\frac{d}{dr}\frac{1}{\epsilon(r)}\,, \tag{10}$$

For Si, with A, B, α, β, and γ denoting material

parameters, the last three in units of a_B^{-1}, the spatial dielectric function is given[13] by

$$\frac{1}{\epsilon(r)} = \frac{1}{\kappa_0} + e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r} . \tag{11}$$

It is the second term on the right-hand side of Eq. (10) that has been neglected by SR. This certainly would also affect their t parameter somewhat. Our $\epsilon(r)$ is somewhat different from the one used by SR, so this might also affect the t parameter somewhat.

Finally, we would like to briefly explain the variational procedure used in our calculations. With the substitution of $\psi = r\phi$, one can rewrite Eq. (3) as

$$\frac{\psi''}{r} + \frac{\kappa'}{\kappa}\frac{\psi'}{r} - \frac{\kappa_0 R_0^{-2}}{\kappa}\frac{\psi}{r} - \kappa\frac{\psi}{r}\frac{d^2}{dr^2}\frac{1}{\epsilon} = 0. \tag{12}$$

An approximate solution of Eq. (11) can be obtained by the variational principle

$$L\{\psi\} = \int_0^\infty \left[-\tfrac{1}{2}\kappa(\psi')^2 - \tfrac{1}{2}\kappa_0 R_0^{-2}\psi^2 - \tfrac{1}{2}\kappa^2\psi^2\frac{d^2}{dr^2}\left(\frac{1}{\epsilon}\right)\right], \tag{13}$$

which has been proposed by Csavinszky and Morrow.[8] That the variational principle is equivalent to the differential equation can easily be seen; denoting the integrand in Eq. (13) by F, substitution of F into the Euler-Lagrange equation,

$$\frac{\partial}{\partial\psi}F - \frac{d}{dr}\frac{\partial}{\partial\psi'}F = 0 , \tag{14}$$

leads to Eq. (12).

Finally, we acknowledge useful discussions with K. R. Brownstein.

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[1]L. M. Scarfone and L. M. Richardson, Phys. Rev. B 22, 982 (1980).

[2]P. Csavinszky, Phys. Rev. B 14, 1649 (1976). In this paper it was believed that the $(\kappa'/\kappa)\phi'$ term of Eq. (1) of the present comment is negligible. The variational parameters obtained in this paper suffer from this defect and, more significantly, from the application of an incorrect boundary condition at the origin.

[3]See Eq. (A13) of Ref. 2.

[4]See Eqs. (7) and (9) of Ref. 2.

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

[6]We note here that in their paper SR give Eqs. (1) and (2) as $\phi'' + (2/r)\phi' + 4\pi\rho/\kappa + (\kappa'/\kappa)\phi = 0$, and $\phi'' + (2/r)\phi' + \kappa^{-1}(\kappa' - \kappa_0/R_0^2)\phi = 0$. These equations are incorrect. We, however, proceed on the assumption that in their calculations they used the correct equation, namely Eq. (3) of this comment. We make this assumption because in an earlier paper by SR [Phys. Rev. B 19, 5139 (1979)] they use the correct equations, namely Eqs. (1) and (2) of this comment.

[7]We use the finite-difference method to integrate Eq. (3) in towards the origin beginning at a large distance. Our results agree with Meyer [J. R. Meyer, Phys. Rev. B 20, 1762 (1979)] when proper account is taken of the distinction between $\epsilon(r)$ and $\kappa(r)$.

[8]P. Csavinszky and R. A. Morrow, Bull. Am. Phys. Soc. 24, 277 (1979).

[9]Using an electron concentration of $n = 10^{20}$ cm^{-3}, an effective mass of $m^* = (6)^{2/3}(m_l m_t^2)^{1/3}$ to account for the six equivalent energy spheroids of Si in k space, and a static dielectric constant of $\kappa_0 = 11.7$, the value of $R_0 = 11.3\, a_0$ is obtained from Eq. (9) of Ref. 2.

[10]R. A. Morrow and P. Csavinszky, Bull. Am. Phys. Soc. 24, 277 (1979).

[11]S. Okuro and M. Azuma, J. Phys. Soc. Jpn. 20, 1099 (1964).

[12]Equation (10) of the present comment is available in the literature [P. Csavinszky Phys. Rev. B 20, 4372 (1979)], though without the explanation presented here.

[13]M. Azuma and K. Shindo, J. Phys. Soc. Jpn. 19, 424 (1964). Concerning two misprints, see Ref. 2.

[14]L. Beauperthuy, M. S. thesis, University of Maine, 1980 (unpublished).