Variational principles for solving nonlinear Poisson equations for the potential of impurity ions in semiconductors with spatially variable dielectric constants

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The theory of the potential of a (point) impurity ion in a semiconductor involves an expansion of the screening-charge density in terms of the impurity-ion potential. In a recent paper, this problem has been reexamined by taking into consideration the spatial variation of the dielectric constant of the host medium. In this paper, the linearized Poisson equation, with the neglect of a small term, has been solved approximately by making use of an equivalent variational principle. In another recent paper, the spatial variation of the dielectric constant has been ignored and variational principles have been formulated for obtaining approximate solutions to nonlinear Poisson equations of any given order in the impurity-ion potential. The present paper aims at the unification of the above two approaches and presents variational principles for obtaining approximate solutions of nonlinear Poisson equations for the potential of an impurity ion which is located in a medium characterized by a spatially variable dielectric constant.

I. INTRODUCTION

In a previous investigation,[1] Dingle's theory[2] of the screening of a (point) impurity ion in semiconductors (characterized by standard energy bands) has been generalized by including in the theory the spatial variation of the dielectric constant of the medium. The linearized Poisson equation, with the neglect of a small term, has been solved approximately by making use of an equivalent variational principle. This procedure resulted in a (donor-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. A blemish of this result lies in the fact that, as the distance from the donor ion goes to zero, the potential remains still scaled by the static dielectric constant of the medium. A subsequent investigation[3] showed that this feature of the impurity-ion potential can be eliminated by a modification of the previous theory.[1] Another investigation[4] succeeded in representing the term neglected[1] in Poisson's equation as an infinite series. It has, subsequently, been possible to show[5] that, at distances larger than Dingle's screening length R_0, the neglected term adds to the impurity-ion potential[1] 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 completely 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.[6,7]

All of the conclusions mentioned above have been reached on the basis of a linearized Poisson equation for a (point) impurity ion embedded in a semiconductor which is characterized by a spatially variable dielectric constant. Another line of investigation[8] focused on solving nonlinear Poisson equations for the potential of a (point) impurity ion that finds itself embedded in a semiconductor which is characterized by its static dielectric constant. (Early attempts to treat this type of a problem have been made by Csavinszky[9] and Adawi.[10]) These types of Poisson equations result from the expansion (in terms of the impurity-ion potential) of the Fermi-Dirac function $\mathfrak{F}_{1/2}$, which appears in the screening-charge density. Use of equivalent variational principles[8] has suggested that the approximate solutions to the nonlinear Poisson equations can be represented as linear combinations of exponentially screened Coulomb potentials (which are scaled by the static dielectric constant of the semiconductor). The use of the variational principles is, however, contingent upon the convergence of the expansion of $\mathfrak{F}_{1/2}$. A formal test of the convergence of the series showed[11] that, in the classical limit, the series does converge at all distances from the donor ion, while, in the degenerate limit, the convergence is assured only beyond a certain distance from the impurity ion (which depends on the Fermi level).

The purpose of the present paper is the unification of the two main approaches.[1,8] Since most of the mathematical details have already been given elsewhere,[1,4,8] Sec. II gives only the salient points of the theory.

II. THEORY

Poisson's equation, for the potential $\phi(r)$ of a (point) donor ion, in a medium of dielectric con-

stant $\kappa(r)$, is of the form[1]

$$\phi'' + \frac{2}{r}\phi' + \frac{4\pi\rho}{\kappa} = -\frac{1}{\kappa}\frac{d\kappa}{dr}\phi', \tag{1}$$

where

$$\rho(r) = 2e_0(2\pi m_n k_B T)^{3/2}\hbar^{-3} \times [\mathfrak{F}_{1/2}(\eta_n) - \mathfrak{F}_{1/2}(\eta_n + e_0\phi/k_B T)] \tag{2}$$

is the screening-charge density (composed of free electrons in a standard conduction band), and

$$\kappa^{-1} = e^{-\alpha r} + A(1 - e^{-\beta r}) + B(1 - e^{-\gamma r}) \tag{3}$$

is the inverse of the spatial dielectric function of the medium.

In Eq. (2), e_0 is the magnitude of the electron charge, m_n is the (scalar) effective mass of the electron, k_B is Boltzmann's constant, and T is the absolute temperature, while the Fermi-Dirac integral $\mathfrak{F}_{1/2}$ is defined[2] by

$$\mathfrak{F}_k(\eta_n) = \frac{1}{k!}\int_0^\infty \frac{x^k\,dx}{e^{x-\eta_n}+1}, \tag{4}$$

where the reduced Fermi level η_n is related to the Fermi level ζ_n by

$$\eta_n = \zeta_n/k_B T. \tag{5}$$

In what follows, the right-hand side of Eq. (1) will be put equal to zero for reasons discussed elsewhere.[1,4,5]

In Eq. (3), the constants A, B, α, β, γ are specific to a given semiconductor and have been obtained by Azuma and Shindo[6] for Si, and by Okuro and Azuma[7] for Ge, with the constraint of

$$A + B = \kappa_0^{-1}, \tag{6}$$

where κ_0 is the static dielectric constant of the semiconductor.

Introducing the function

$$\psi(r) = r\phi, \tag{7}$$

Eq. (1) can be written

$$\psi'' + 4\pi\rho/\kappa = 0. \tag{8}$$

Expanding $\mathfrak{F}_{1/2}(\eta_n + e_0\phi/k_B T)$ in Eq. (2) in terms of $e_0\phi/k_B T$, and making use of the relation[2]

$$\mathfrak{F}_k'(\eta_n) = \mathfrak{F}_{k-1}(\eta_n), \tag{9}$$

Eq. (8) is brought to the form

$$\psi'' - R_0^{-2}\psi - \kappa_0 R_0^{-2}\psi(e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r}) - \epsilon_1 R_0^{-2}(\psi^2/r) - \epsilon_2 R_0^{-2}(\psi^3/r^2) - \epsilon_3 R_0^{-2}(\psi^4/r^3) - \cdots - \epsilon_1 R_0^{-2}\kappa_0(\psi^2/r)(e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r}) - \epsilon_2 R_0^{-2}\kappa_0(\psi^3/r^2)(e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r}) - \epsilon_3 R_0^{-2}\kappa_0(\psi^4/r^3)(e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r}) - \cdots = 0, \tag{10}$$

where R_0, a screening length introduced by Dingle,[2] is defined by

$$R_0^{-2} = [16\pi^2 e_0^2 m_n^{3/2}(2\pi k_B T)^{1/2}/\kappa_0\hbar^3]\mathfrak{F}_{-1/2}(\eta_n), \tag{11}$$

while the quantities $\epsilon_1, \epsilon_2, \epsilon_3, \ldots$ stand[8] for

$$\epsilon_1 = \frac{1}{2!}\frac{e_0}{k_B T}\frac{\mathfrak{F}_{-3/2}(\eta_n)}{\mathfrak{F}_{-1/2}(\eta_n)}, \quad \epsilon_2 = \frac{1}{3!}\left(\frac{e_0}{k_B T}\right)^2\frac{\mathfrak{F}_{-5/2}(\eta_n)}{\mathfrak{F}_{-1/2}(\eta_n)}, \quad \epsilon_3 = \frac{1}{4!}\left(\frac{e_0}{k_B T}\right)^3\frac{\mathfrak{F}_{-7/2}(\eta_n)}{\mathfrak{F}_{-1/2}(\eta_n)}, \quad \cdots. \tag{12}$$

The central problem is to solve Eq. (10), which is the (approximate) nonlinear Poisson equation for the potential of a (point) impurity ion in a medium of variable dielectric constant. This we wish to do by making use of an equivalent variational principle. To this end, consider the functional

$$L\{\psi\} = \int_{r_0}^\infty F(\psi, \psi', r)\,dr, \tag{13}$$

where ψ is a trial function (which depends on a number of appropriately chosen parameters), and the lower limit of integration r_0 is a constant (whose choice will be discussed later).

The task is now the finding of an expression for F, in such a manner, that upon substituting F into the Euler-Lagrange equation[12]

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

one obtains Eq. (10). It is seen that this is the case if F is chosen as

$$F = -\tfrac{1}{2}(\psi')^2 - \tfrac{1}{2}R_0^{-2}\psi^2 - \tfrac{1}{2}\kappa_0 R_0^{-2}e^{-\alpha r}\psi^2 + \tfrac{1}{2}\kappa_0 R_0^{-2}Ae^{-\beta r}\psi^2 + \tfrac{1}{2}\kappa_0 R_0^{-2}Be^{-\gamma r}\psi^2$$
$$- \tfrac{1}{3}\epsilon_1 R_0^{-2}(\psi^3/r) - \tfrac{1}{4}\epsilon_2 R_0^{-2}(\psi^4/r^2) - \tfrac{1}{5}\epsilon_3 R_0^{-2}(\psi^5/r^3) - \cdots$$
$$- \tfrac{1}{3}\epsilon_1 R_0^{-2}\kappa_0 e^{-\alpha r}(\psi^3/r) + \tfrac{1}{3}\epsilon_1 R_0^{-2}\kappa_0 Ae^{-\beta r}(\psi^3/r) + \tfrac{1}{3}\epsilon_1 R_0^{-2}\kappa_0 Be^{-\gamma r}(\psi^3/r) - \tfrac{1}{4}\epsilon_2 R_0^{-2}\kappa_0 e^{-\alpha r}(\psi^4/r^2)$$
$$+ \tfrac{1}{4}\epsilon_2 R_0^{-2}\kappa_0 Ae^{-\beta r}(\psi^4/r^2) + \tfrac{1}{4}\epsilon_2 R_0^{-2}\kappa_0 Be^{-\gamma r}(\psi^4/r^2) - \tfrac{1}{5}\epsilon_3 R_0^{-2}\kappa_0 e^{-\alpha r}(\psi^5/r^3)$$
$$+ \tfrac{1}{5}\epsilon_3 R_0^{-2}\kappa_0 Ae^{-\beta r}(\psi^5/r^3) + \tfrac{1}{5}\epsilon_3 R_0^{-2}\kappa_0 Be^{-\gamma r}(\psi^5/r^3) - \cdots . \quad (15)$$

The next step consists of choosing a trial function $\psi(\mu_1, \mu_2, \ldots)$, where $\mu_1, \mu_2, \ldots$ are parameters to be determined from the conditions

$$\left.\frac{\partial L(\mu_1, \mu_2, \ldots)}{\partial \mu_1}\right|_{R_0=\text{const}} = 0,$$

$$\left.\frac{\partial L(\mu_1, \mu_2, \ldots)}{\partial \mu_2}\right|_{R_0=\text{const}} = 0, \quad (16)$$

$\cdots$

As to the boundary conditions that ψ must obey, the following are suggested:

$$\psi(0) = e_0 \quad (17)$$

and

$$\psi(\infty) = 0. \quad (18)$$

These assure us that the potential ϕ, at small and large distances from the impurity ion, behaves as

$$\phi(r \to 0) \quad (19a)$$

and

$$\phi(r \to \infty) \quad (19b)$$

In Ref. 1, Dingle's boundary condition $\phi(r \to 0) = e_0/\kappa_0 r$ has been used. The goal at that time consisted in incorporating the spatial variation of the dielectric constant into Poisson's equation for the impurity-ion potential. [The change of $\kappa(r)$ with r is more rapid in Si than it is in Ge, as can be seen from the graphs given in Refs. 6 and 7. In both cases, however, $\kappa(r)$ reaches the value of κ_0 in a distance ($\sim 8a_B$ for Si and $\sim 5a_B$ for Ge) which is smaller than the lattice constant.] The realization that, in addition to the correct Poisson equation, the behavior of the trial function in the immediate vicinity of the impurity ion may affect it even at large distances from the impurity ion motivated the work of Ref. 3.

The trial function suggested there for the potential of a donor ion is of the form

$$\phi^{(1)} = (e_0 e^{-\lambda_1^{(1)} r}/\kappa_0 r)[1 + (\kappa_0 - 1)e^{-\lambda_2^{(1)} r}], \quad (20)$$

where $\lambda_1^{(1)}$ and $\lambda_2^{(1)}$ are variational parameters. It is easily seen that Eq. (20) satisfies the boundary conditions in Eqs. (19a) and (19b). The trial function in Eq. (20) is pertinent to a Poisson equation that is linear in the impurity-ion potential. In the work[8] that ignored the spatial variation of the dielectric constant but considered Poisson equations which are quadratic, cubic, etc., in the impurity-ion potential, the suggestion has been made that the trial potentials for these cases should be represented as linear combinations of two exponentially screened Coulomb potentials, three exponentially screened Coulomb potentials, etc.

Following this line of reasoning, the trial potentials for the quadratic, cubic, etc., Poisson equations, as given by Eqs. (7) and (10), might be constructed as

$$\phi^{(2)} = (e_0/\kappa_0 r)(C^{(2)}e^{-\lambda_1^{(2)} r} + D^{(2)}e^{-\lambda_2^{(2)} r}) \times [1 + (\kappa_0 - 1)e^{-\lambda_3^{(2)} r}], \quad (21)$$

$$\phi^{(3)} = (e_0/\kappa_0 r)(C^{(3)}e^{-\lambda_1^{(3)} r} + D^{(3)}e^{-\lambda_2^{(3)} r} + E^{(3)}e^{-\lambda_3^{(3)} r}) \times [1 - (\kappa_0 - 1)e^{-\lambda_4^{(3)} r}], \quad (22)$$

$\cdots$,

where the parameters $C^{(2)}$ and $D^{(2)}$ in Eq. (21) are subject to the constraint

$$C^{(2)} + D^{(2)} = 1, \quad (23)$$

while the parameters $C^{(3)}$, $D^{(3)}$, and $E^{(3)}$ in Eq. (22) are subject to that of

$$C^{(3)} + D^{(3)} + E^{(3)} = 1, \quad (24)$$

etc. The constraints in Eqs. (23) and (24) are necessary if Eq. (19a) is to be satisfied. In view of the above, the quantity L in Eq. (13) becomes a function of two parameters ($\lambda_1^{(1)}, \lambda_2^{(1)}$) when dealing with the linear Poisson equation, a function of four parameters ($C^{(2)}, \lambda_1^{(2)}, \lambda_2^{(2)}, \lambda_3^{(2)}$) when dealing with the quadratic Poisson equation, and a function of six parameters ($C^{(3)}, D^{(3)}, \lambda_1^{(3)}, \lambda_2^{(3)}, \lambda_3^{(3)}, \lambda_4^{(3)}$) when dealing with the cubic Poisson equation, etc.

As has been shown[8] before, the integrals that result from the substitution of Eq. (15) into Eq. (13) are of two types. The first type consists of integrals that can be evaluated without any difficulty. The second type consists of integrals whose denominator contains $1/r^2$, $1/r^3, \ldots$, etc. This latter type of integrals can be reduced, upon partial integration, to integrals which give no trouble, and to integrals which can be expressed in terms of the exponential integral, defined[13] by

$$-E_i(-\xi) = \int_{\xi}^{\infty} \frac{e^{-u}}{u}\, du. \tag{25}$$

All of these integrals contain r_0, the lower limit of integration in Eq. (13). The choice of this quantity should be such that the validity of the expansion in Eq. (10) is assured. The choice for r_0 is, necessarily, coupled with some uncertainty. It has been shown[11] that, in the limit of complete degeneracy, the expansion of $\mathfrak{F}_{1/2}(\eta_n + e_0\phi/k_BT)$ is assured for distances at which $e_0\phi(r)/\zeta_n < 1$. In the completely nondegenerate limit, no restriction on the expansion of $\mathfrak{F}_{1/2}[\eta_n + e_0\phi(r)/k_BT]$ has been found.[11] In view of this finding, at least in the degenerate limit, one may carry through the variational calculation with an assumed r_0 value [Eq. (13) can be evaluated with any value of r_0], and then check on the validity of the $e_0\phi(r)/\zeta_n < 1$ condition.

Once $L\{\psi\} = L(\mu_1, \mu_2, \ldots)$ is obtained, its extreme value, in principle, is determined from Eqs. (16). In practice, this might proceed via two routes. The parameters $\mu_1, \mu_2, \ldots$ (appearing in ξ) are either such that series expansions[14] for $-\mathrm{Ei}(-\xi)$ can be used, or they are such that tables[15] of this function must be consulted.

III. CONCLUDING REMARKS

It is anticipated that the impurity-ion potential to be obtained from the considerations of this paper might find use in theories of ionized-impurity scattering. Theoretical treatments of this scattering process, such as the well-known theories of Conwell and Weisskopf,[16] of Brooks and Herring,[17] or the less often used partial wave theories of Blatt,[18] of Csavinszky,[19] and of Krieger and Strauss,[20] are all based on a potential that is devoid of the refinements of the potential suggested in this paper. The same is true with regard to corrections to the Brooks-Herring[17] mobility formula, which have been calculated by Moore,[21] by Moore and Ehrenreich,[22] and by Luong and Shaw.[23]

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