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

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In the above-named paper, a simplified form of the nonlinear Poisson equation for the impurity-ion potential has been solved approximately by making use of an equivalent variational principle. The difference between the exact and the simplified nonlinear Poisson equations is a term involving the derivative of the potential and the derivative of the spatially variable dielectric constant. The purpose of the present paper is the presentation of a more general variational principle, by which one might obtain an approximate solution of the exact nonlinear Poisson equation.

## I. INTRODUCTION

A linearized theory of the screening of (point) impurity ions in semiconductors characterized by a spatially variable dielectric constant $\kappa(r)$ has been given in a recent paper.[1] This was followed by another work[2], in which the nonlinear theory of the screening of impurity ions has been established.[3]

In Refs. 1 and 2, a simplified form of Poisson's equation for the donor-ion potential $\phi(r)$ has been solved approximately by making use of an equivalent variational principle. The difference between the exact and the simplified (linear or nonlinear) Poisson equations is a term which involves the derivative of the potential and the derivative of the spatially variable dielectric constant. In another recent paper,[4] a more general variational principle than the one presented in Ref. 1 has been arrived at by which the exact linearized Poisson equation might be solved approximately. The purpose of the present paper is the generalization of the variational principle used in Ref. 2, by which one might obtain an approximate solution of the exact nonlinear Poisson equation.

## II. THEORY

Poisson's equation for the potential of a charged donor ion has been found[5] to be of the form

$$\nabla^2\phi+\frac{4\pi\rho}{\kappa}+\frac{\vec{\nabla}\kappa\cdot\vec{\nabla}\phi}{\kappa}=0\,, \tag{1}$$

where $\rho(r)$ is the density of the screening charge (composed of mobile electrons), and $r$ is the distance from the fixed point charge.

In the nonlinear theory,[2] $\rho$ is related[6] to $\phi$ by

$$\rho=2e_0(2\pi m^*k_BT)^{3/2}h^{-3}\left[\mathfrak{F}_{1/2}(\eta_\nu)-\mathfrak{F}_{1/2}\left(\eta_\nu+\frac{e_0\phi}{k_BT}\right)\right], \tag{2}$$

where $e_0$ is the magnitude of the electron charge, $m^*$ is a scalar effective mass,[7] $k_B$ is Boltzmann's constant, $T$ is the absolute temperature, and the Fermi-Dirac integral $\mathfrak{F}_{1/2}$ is defined[8] by

$$\mathfrak{F}_k(\eta_\nu)=\frac{1}{k!}\int_0^\infty\frac{x^k dx}{e^{x-\eta_\nu}+1}\,, \tag{3}$$

with $\eta_\nu$ denoting the reduced Fermi level, which is related to the Fermi level $\zeta_\nu$ by

$$\eta_\nu=\frac{\zeta_\nu}{k_BT}\,. \tag{4}$$

Expanding $\mathfrak{F}_{1/2}(\eta_\nu+e_0\phi/k_BT)$ in powers of $e_0\phi/k_BT$, and making use of the relation[8]

$$\mathfrak{F}_k'(\eta_\nu)=\mathfrak{F}_{k-1}(\eta_\nu)\,, \tag{5}$$

one finds that Eq. (2) becomes

$$\rho=-\frac{2e_0(2\pi m^*k_BT)^{3/2}}{h^3}\left[\left(\frac{e_0}{k_BT}\right)\mathfrak{F}_{-1/2}(\eta_\nu)\phi+\frac{1}{2!}\left(\frac{e_0}{k_BT}\right)^2\mathfrak{F}_{-3/2}(\eta_\nu)\phi^2+\frac{1}{3!}\left(\frac{e_0}{k_BT}\right)^3\mathfrak{F}_{-5/2}(\eta_\nu)\phi^3+\cdots\right]. \tag{6}$$

Introducing a screening length[8] $R_0$ by

$$R_0^{-2}=\frac{16\pi^2e_0^2m^{*3/2}(2\pi k_BT)^{1/2}}{\kappa_0h^3}\mathfrak{F}_{-1/2}(\eta_\nu)\,, \tag{7}$$

where $\kappa_0$ is the static dielectric constant of the medium, and adopting Cartesian coordinates, substitution of Eq. (6) into Eq. (1) leads to

$$\kappa(\phi_{xx}+\phi_{yy}+\phi_{zz})-\kappa_0\left(\frac{k_BT}{e_0}\right)R_0^{-2}\left[\left(\frac{e_0}{k_BT}\right)\phi+\frac{1}{2!}\left(\frac{e_0}{k_BT}\right)^2\frac{\mathfrak{F}_{-3/2}(\eta_\nu)}{\mathfrak{F}_{-1/2}(\eta_\nu)}\phi^2+\frac{1}{3!}\left(\frac{e_0}{k_BT}\right)^3\frac{\mathfrak{F}_{-5/2}(\eta_\nu)}{\mathfrak{F}_{-1/2}(\eta_\nu)}\phi^3+\cdots\right]$$
$$+\kappa_x\phi_x+\kappa_y\phi_y+\kappa_z\phi_z=0\,, \tag{8}$$

where the subscripts on $\phi$ and $\kappa$ refer to the appropriate partial derivatives of these quantities.

Defining

$$\delta_1=\frac{1}{2!}\left(\frac{e_0}{k_BT}\right)\frac{\mathfrak{F}_{-3/2}(\eta_\nu)}{\mathfrak{F}_{-1/2}(\eta_\nu)}\,,$$
$$\delta_2=\frac{1}{3!}\left(\frac{e_0}{k_BT}\right)^2\frac{\mathfrak{F}_{-5/2}(\eta_\nu)}{\mathfrak{F}_{-1/2}(\eta_\nu)}\,, \tag{9}$$

one can express Eq. (8) as

$$\kappa(\phi_{xx}+\phi_{yy}+\phi_{zz})-\kappa_0R_0^{-2}(\phi+\delta_1\phi^2+\delta_2\phi^3+\cdots)+\kappa_x\phi_x+\kappa_y\phi_y+\kappa_z\phi_z=0\,. \tag{10}$$

Equation (10) represents the exact nonlinear Poisson equation in Cartesian coordinates. The difference between Eq. (10) and the simplified nonlinear Poisson equation discussed in Ref. 2 is the last three terms in Eq. (10).

The next task consists now in finding a variational principle by which Eq. (10) might be solved approximately. To this end, one can consider the variational principle

$$L\{\phi\}=\int\int\int G(\phi,\phi_x,\phi_y,\phi_z,x,y,z)\,dx\,dy\,dz\,, \tag{11}$$

where the limits of integration will be discussed later.

As is known,[9] the function $\phi$ which makes $L\{\phi\}$ stationary must satisfy the Euler-Lagrange equation

$$\frac{\partial G}{\partial\phi}-\frac{\partial}{\partial x}\frac{\partial G}{\partial\phi_x}-\frac{\partial}{\partial y}\frac{\partial G}{\partial\phi_y}-\frac{\partial}{\partial z}\frac{\partial G}{\partial\phi_z}=0\,. \tag{12}$$

To proceed, one has to find an expression for $G$ in such a manner that, upon substituting $G$ into Eq. (12), one obtains Eq. (10). A little reflection shows that this requirement is achieved if $G$ is chosen as

$$G=-\tfrac{1}{2}\kappa(\phi_x^2+\phi_y^2+\phi_z^2)$$
$$-\kappa_0R_0^{-2}(\tfrac{1}{2}\phi^2+\tfrac{1}{3}\delta_1\phi^3+\tfrac{1}{4}\delta_2\phi^4+\cdots)\,. \tag{13}$$

Passing now to spherical polar coordinates, and considering that in the case of spherical symmetry

$$\vec{\nabla}\phi=\phi'\hat{e}_r\,, \tag{14}$$

where the prime on $\phi$ denotes the derivative of $\phi$ with respect to $r$, with $\hat{e}_r$ denoting a unit vector, and considering the relation

$$\vec{\nabla}\phi\cdot\vec{\nabla}\phi=\phi_x^2+\phi_y^2+\phi_z^2\,, \tag{15}$$

one can cast Eq. (13) into the form

$$G=-\tfrac{1}{2}\kappa(\phi')^2-\kappa_0R_0^{-2}(\tfrac{1}{2}\phi^2+\tfrac{1}{3}\delta_1\phi^3+\tfrac{1}{4}\delta_2\phi^4+\cdots)\,. \tag{16}$$

Considering that

$$dx\,dy\,dz=4\pi r^2dr\,, \tag{17}$$

substitution of Eq. (16) into Eq. (11), upon use of Eq. (17), results in

$$L\{\phi\}=4\pi\int_{r_0}^{\infty}(Gr^2)\,dr\,, \tag{18}$$

where an appropriate choice for the lower limit of integration $r_0$ has been discussed in detail in Ref. 4.

Equation (18) is the variational principle in spherical polar coordinates by which Eq. (1) might be solved approximately. To see this, one only has to substitute $(Gr^2)$ into the appropriate Euler-Lagrange equation[9]

$$\frac{\partial}{\partial\phi}(Gr^2)-\frac{d}{dr}\frac{\partial}{\partial\phi'}(Gr^2)=0\,, \tag{19}$$

and find that the result is

$$\phi''+\frac{2}{r}\phi'-\frac{\kappa_0R_0^{-2}}{\kappa}(\phi+\delta_1\phi^2+\delta_2\phi^3+\cdots)+\frac{\kappa'}{\kappa}\phi'=0\,, \tag{20}$$

which is Eq. (10) in spherical polar coordinates.

To complete the discussion, the spatially variable dielectric constant $\kappa(r)$ has yet to be defined. In Refs. 1 and 2, this quantity has been taken equal to the spatial dielectric function of a particular semiconductor. It has, however, been shown elsewhere[4] that such an identification of the spatially variable dielectric constant with the spatial dielectric function is permissible only in the immediate vicinity of the impurity ion and at large distances from it. In the intermediate distance region, the spatially variable dielectric constant can be expressed[4] in terms of the spatial dielec-

tric function $\epsilon(r)$ by

$$\frac{1}{\kappa}=\frac{1}{\epsilon}+r\left(\frac{\epsilon'}{\epsilon}\right)\frac{1}{\epsilon}, \tag{21}$$

where the prime on $\epsilon$ denotes the derivative of $\epsilon$ with respect to $r$.

## III. CONCLUSIONS

It is hoped that the variational principle presented in this paper might find application in obtaining an approximate solution of the nonlinear Poisson equation for the donor-ion potential. A variational solution to this problem appears to be advantageous in light of the fact that it has recently been shown[10] that nonlinear Poisson equations [both in a medium characterized by $\kappa_0$ or in a medium characterized by $\kappa(r)$] in the vicinity of a donor ion reduce to the Thomas-Fermi (TF) equation. The solution of the TF equation for small values of $r$ is known.[11] The large-$r$ solution of the nonlinear Poisson equations is also known. It is the Dingle[8] result, an exponentially screened Coulomb potential. This can be seen from Eq. (20). At large distances from the donor ion $\phi^2<\phi$, $\phi^3<\phi^2$, etc., and $\kappa'=0$. In this case, Eq. (20) reduces to the Poisson equation discussed by Dingle. What is not known is the behavior of the donor-ion potential between the small-$r$ and the large-$r$ limits. It is hoped that by making use of the variational principle advocated here (and in Ref. 3), one might construct a trial potential which incorporates both the required small-$r$ and the large-$r$ behavior of the potential.

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[3]A nonlinear theory of the same problem, in media characterized by a static dielectric constant $\kappa_0$, has also been recently advanced [P. Csavinszky, Phys. Rev. B 14, 4483 (1976)].
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[5]See. Eq. (A9) of Ref. 1.
[6]See Eq. (2) of Ref. 2.
[7]If the semiconductor is of a multivalley type, such as Si or Ge, than for a particular valley, $m^*$ should be replaced by $(m_l m_t^2)^{1/3}$, where $m_l$ is the longitudinal and $m_t$ is the transverse effective mass.
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