

Solution of a nonlinear Poisson's equation for the potential of impurity ions in semiconductors with a spatially variable dielectric constant by an equivalent variational method

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A correct knowledge of the screening potential in heavily doped semiconductors is highly desirable for analyzing various electronic engineering problems. In this paper a method for the solution of a nonlinear Poisson's equation in the framework of an equivalent variational approach is presented. Strengths and weaknesses of the earlier methods, including those of Csavinszky and co-workers, have been discussed in some detail. On the basis of a comparison of the present method with the earlier ones, it is felt that the present one is very promising, and perhaps more general and unified than most, if not all, other methods available in the literature.

I. INTRODUCTION

The scattering of the mobile charge carriers by ionized impurity atoms is one of the most important scattering processes in heavily doped semiconductors. Almost all of the theoretical treatments¹ of this scattering process make use of the potential that results from the screening of impurity ions by mobile charge carriers. This potential finds other applications as well. For example, it is noted that the screening potential is highly useful for estimating band-gap narrowing²⁻⁴ in electronic devices with heavily doped semiconductor regions. Calculation of depletion layer width and junction depletion capacitance for a heavily doped *p-n* junction is based on the same screening potential.^{5,6} A knowledge of depletion layer width is vital to the formulation of important parameters such as Early voltage of bipolar transistors.^{7,8} An accurate analytical form for screening potential is desirable for the performance analyses of metal-oxide-semiconductor field-effect transistors (MOSFET's).⁹ Because of such an enormous importance of screening potential for the evaluation and analyses of parameters of electronic devices, a number of researchers,¹¹⁻²³ including Csavinszky and co-workers,¹²⁻²² attempted to address various aspects of this problem in some details. In a series of papers Csavinszky and co-workers made use of an equivalent variational method to develop a modified formula for the screened Coulomb potential, taking, for example, spatial variation of dielectric constant, and higher powers of the expansion of Fermi-Dirac integral of order $\frac{1}{2}$, into account. Despite great successes, the method seems to have some shortcomings. For example, when the spatial dependence of the dielectric constant and the higher powers of the expansion of Fermi-Dirac integral of order $\frac{1}{2}$ are taken into account, the modified Poisson's equation becomes extremely complicated, and almost intractable for extracting useful informations [see, for example, Eq. (15) of Ref. 15]. Even in this form, it remains inadequate for small-distance behavior.¹⁷ Our aim in this investigation is to propose an alternative

method, which in the framework of the same powerful equivalent variational technique of mathematics,²⁴ would be simpler, and would yet lead to a more accurate and generalized screening potential.

II. THEORETICAL METHOD

Let us consider an *n*-type (uncompensated) heavily doped semiconductor region characterized by spatially variable dielectric constant $\epsilon(r)$. In such a semiconductor one excess electron is provided by each donor atom. The Poisson's equation, for the potential $\varphi(r)$ of this semiconductor region, would be given by¹²

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

where r is the spherical polar coordinate, and $\rho(r)$ is the density of screening charge. Let e_0 be the electronic charge, m^* the isotropic effective electron mass, T the absolute temperature, k the Boltzmann constant, and h is Planck's constant. The charge density $\rho(r)$ may be expressed as

$$\rho(r) = A [F_{1/2}(\eta) - F_{1/2}(\eta + e_0\varphi/kT)], \quad (2)$$

where η is the reduced Fermi level, $\eta = (E_F - E_c)/kT$, E_F is the Fermi energy, and E_c is the lowest edge of the conduction band. The parameter A is defined as

$$A = \frac{2e_0(2\pi m^* kT)^{3/2}}{h^3}. \quad (3)$$

The Fermi-Dirac integral of order j given, in general, by

$$F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{z^j dz}{1 + e^{z-\eta}}, \quad (4a)$$

does not possess analytic closed-form expressions for any of the interesting $j \neq 0$ members of Eq. (4a). An approximate expression for $F_{1/2}(\eta)$ may be given by

$$F_{1/2}(\eta) = \sum_{\nu=0}^{10} a_\nu \eta^\nu, \quad (4b)$$

TABLE I. Various parameters a_v ($v=0-10$) used to define Eq. (4b).

Parameter	Value of the parameter
a_0	0.677 36
a_1	0.547 14
a_2	0.168 89
a_3	$0.125\ 38 \times 10^{-1}$
a_4	$-0.282\ 12 \times 10^{-2}$
a_5	$-0.970\ 32 \times 10^{-5}$
a_6	$0.514\ 83 \times 10^{-4}$
a_7	$-0.636\ 48 \times 10^{-5}$
a_8	$3.618\ 30 \times 10^{-7}$
a_9	$-1.023\ 60 \times 10^{-8}$
a_{10}	$1.164\ 90 \times 10^{-10}$

where a_v ($v=0-10$) are suitable parameters listed in Table I. Variation of $F_{1/2}(\eta)$ with η as calculated from Eq. (4b) is shown in Fig. 1. For the sake of comparison, exact values²⁵ of $F_{1/2}(\eta)$ for various values of η are also presented in the figure. From this figure it may be noted that the calculated results are in very good agreement with the exact results, and that the range covered by η corresponds both to nondegenerate and highly degenerate levels of the material. The average percent error

$$\Delta\eta = \frac{[\eta(\text{exact}) - \eta(\text{calc})]100\%}{\eta(\text{exact})} \tag{4c}$$

for the most values of η in the range $-4 \leq \eta \leq 20$ is less than 0.02. Values of η for $\eta < 0.0$ are very small, and hence a small deviation of the calculated results from the exact ones causes a very large percent error. Because of this, although $\Delta\eta$ is about 2.0 for $\eta = -2.0$, and to some extent higher for $\eta \leq -4.0$, it should not be taken very seriously.

With the help of Eq. (4b), the screening charge density of Eq. (2) may easily be simplified to

$$\rho(r) = -A \sum_{n=1}^{10} v_n [\varphi(r)]^n, \tag{5}$$

where v_n for $n = 1, 2, 3$, etc. may be given by

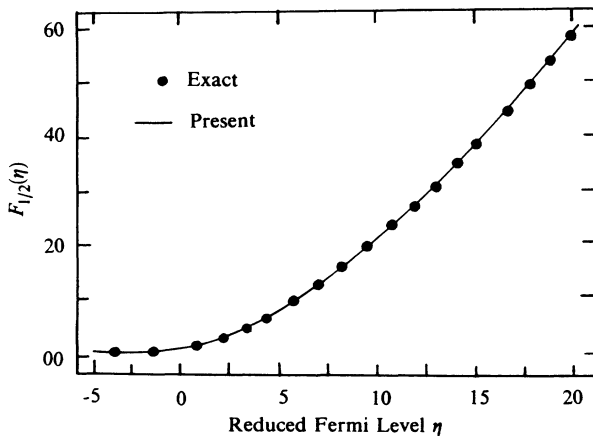


FIG. 1. Comparison of the fitted and exact values of the Fermi-Dirac integral of order $\frac{1}{2}$ as a function of the reduced Fermi level η .

$$v_n = \sum_{\nu=n}^{10} {}^{\nu}C_n a_{\nu} \eta^{\nu-n} s^n, \tag{6}$$

with ${}^{\nu}C_n$ ($n = 1, 2, 3$, etc.) are binomial coefficients

$${}^{\nu}C_n = \frac{\nu!}{n!(\nu-n)!} \tag{7a}$$

and

$$s = \frac{e_0}{kT}. \tag{7b}$$

If we make a substitution $\psi(r) = r\varphi(r)$, then with the help of Eq. (5), Eq. (1) may be rearranged to

$$\frac{d^2\psi}{dr^2} + \frac{\epsilon'}{\epsilon} \frac{d\psi}{dr} - \left[\frac{\epsilon'}{\epsilon r} + \frac{4\pi A v_1}{\epsilon} \right] \psi - \frac{4\pi A}{\epsilon} \sum_{n=2}^{10} \frac{v_n \psi^n}{r^{n-1}} = 0, \tag{8}$$

where $\epsilon' = d\epsilon/dr$.

For the sake of convenience, let us define the following terms:

$$R(r) = \frac{\epsilon'(r)}{\epsilon(r)}, \tag{9a}$$

$$T(r) = \frac{\epsilon'}{\epsilon r} + \frac{4\pi A v_1}{\epsilon}. \tag{9b}$$

Let us also assume that $\psi = \alpha\phi$, and that

$$\alpha(r) = \exp \left[- \int_0^r \frac{R(r)}{2} dr \right]. \tag{9c}$$

An alternate form of Eq. (9c) would be $\alpha = \epsilon^{-1/2}$. Equation (9) allows Eq. (8) to be rewritten as

$$\frac{d^2\phi}{dr^2} + U(r)\phi - \frac{4\pi A}{\epsilon} \sum_{n=2}^{10} \frac{v_n \alpha^{n-1} \phi^n}{r^{n-1}} = 0, \tag{10}$$

with $U(r)$ defined by

$$U(r) = \frac{1}{\alpha} \frac{d^2\alpha}{dr^2} + \frac{R(r)}{\alpha} \frac{d\alpha}{dr} - T(r). \tag{11}$$

Equation (10) may be called the modified Poisson's equation, which is a second-order differential equation with variable coefficients. This equation is similar to Eq. (21) of Csavinsky,¹³ except that the coefficients for the latter are constant, instead of being variable as the former. In order to solve it by the equivalent variational method, we consider the functional

$$L[\phi] = \int_{r_0}^{\infty} F(\phi, \phi', r) dr, \tag{12}$$

where ϕ is a trial function and $\phi' = (d\phi/dr)$. The parameter r_0 is a constant, the value of which depends on the nature of the problem. It will be discussed later. Let us now choose F as

$$F = -\frac{1}{2}(\phi')^2 + \frac{1}{2}U(r)\phi^2 - \frac{4\pi A}{\epsilon} \sum_{n=2}^{10} \frac{v_n \alpha^{n-1} \phi^{n+1}}{r^{n-1} (n+1)}. \tag{13}$$

The expression for F in Eq. (13) is such that when it is substituted into the Euler-Lagrange equation

$$\frac{\partial}{\partial \phi} F - \frac{\partial}{\partial r} \frac{\partial}{\partial \phi'} F = 0, \quad (14)$$

the modified Poisson's equation as given by Eq. (10) would result.

The very success of the present procedure would rest on the judicious choice of the final form for ϕ . As a search for this form for ϕ we examine Eq. (8). From this equation it is apparent that had the dielectric constant of the medium been spatially invariable, and $F_{1/2}(\eta)$ of Eq. (4b) been estimated more approximately, taking only the linear term into account, Eq. (8) would reduce essentially to the form obtained by Dingle.¹¹ This indicates that the terms containing ϵ' and r^{-1} represent the perturbation terms, and that the solution of Eq. (10) would be practically the same as the Dingle potential. So $\phi(r)$ may be assumed to be of the form

$$\phi(r) = Ce^{-ar} + De^{-br}, \quad (15)$$

where C and D are the parameters to be determined by considering the first one of the Dingle boundary conditions

$$\phi(0) = e_0/\epsilon_0, \quad (16a)$$

$$\phi(\infty) = 0, \quad (16b)$$

and where a and b are real and positive. Note that ϵ_0 of Eq. (16a) is the static dielectric constant of the medium, $\epsilon(r) = \epsilon_0$ for r tending to infinity. Equations (15) and (16a) give $D = C - 1$, suggesting that the functional $L[\phi]$ is a function of C , a , and b :

$$L[\phi] = L(C, a, b). \quad (17)$$

If we assume that

$$L[\phi] = L_1 + L_2 + L_3, \quad (18)$$

$$L_1 = \frac{1}{2} \int_{r_0}^{\infty} U(r) \{ Cae^{-ar} + (1-C)be^{-br} \}^2 dr, \quad (19)$$

$$L_2 = -\frac{1}{2} \int_{r_0}^{\infty} \left\{ \frac{d}{dr} [Ce^{-ar} + (1-C)e^{-br}]^2 \right\} dr, \quad (20)$$

$$L_3 = -4\pi A \int_{r_0}^{\infty} \sum_{n=2}^{10} \frac{v_n \alpha^{n-1}}{\epsilon(r)r^{n-1}} [Ce^{-ar} + (1-C)e^{-br}]^n dr, \quad (21)$$

the final task would be the extremalization (e.g., maximization or minimization) of Eq. (18) as follows:

$$F_1(a, b, C) \equiv \frac{\partial L}{\partial C} = 0, \quad F_2(a, b, C) \equiv \frac{\partial L}{\partial a} = 0, \quad (22)$$

$$F_3(a, b, C) \equiv \frac{\partial L}{\partial b} = 0.$$

This extremalization may be carried out by numerical method, which would yield optimum values of C , a , and b , and thus define the screening potential Eq. (15). The evaluation of the integrals would necessitate a knowledge of r_0 . The number of electrons per unit volume surrounding a donor ion may be given by

$$n_e = AF_{1/2}[\eta + e_0\phi(r)/kT], \quad (23)$$

and the screening length R_0 by

$$R_0^{-2} = \frac{4\pi e_0^2 m^* (2m^* \pi kT)^{1/2}}{\epsilon_0 h^3} F_{-1/2}(\eta), \quad (24)$$

with m^* to be the (isotropic) effective mass of electrons.

This distance R_0 of electrons that surround the donor ion would be shortest when the semiconductor is very degenerate. One possible condition for achieving this degeneracy would be to choose r_0 to be that value of r at which

$$\eta = e_0\phi(r)/kT \quad (25)$$

in the expansion of the Fermi-Dirac integral of Eq. (23). An alternate condition would be to equate r_0 to that value of R_0 that corresponds to the highest possible doping level of a semiconductor, and which yet does not lead it to exhibit a metallic character. In the case of silicon, for example, with n -type doping level $N_d = 10^{20} \text{ cm}^{-3}$, R_0^{-1} would be about 0.17 \AA^{-1} .

In order to determine a , b , and C , we may first employ Eqs. (18)–(21) to calculate $\partial L/\partial a$, $\partial L/\partial b$, and $\partial L/\partial C$. When $\partial L/\partial C$ is equated to zero, we obtain C as a function of a and b . This allows us to obtain two transcendental equations

$$F_2(a, b) = 0, \quad (26a)$$

$$F_3(a, b) = 0, \quad (26b)$$

as functions of a and b only. Next, starting with a certain lowest value of b (for example, $b_0 \equiv b = 0.0001$), we choose a series of values of b , viz., $b_1 = (b + \Delta b)$, $b_2 = (b + 2\Delta b)$, $b_3 = (b + 3\Delta b)$, ..., $b_m = (b + m\Delta b)$, etc., where, for example, $\Delta b = 0.0001$, and determine $a_X \equiv a$ from Eq. (26a), and $a_Y \equiv a$ from Eq. (26b) for each of these values of b . The procedure of incrementing b and of determining a_X and a_Y for each incremented value of b , should continue until a_X and a_Y corresponding to a certain incrementation becomes almost identical. Thus we obtain a and b . Once a and b are known, the value of C can be determined very easily.

The differential equation (10), which is dealt with to obtain the screening potential $\phi(r)$, covers the interval $0 \leq r \leq \infty$. This is reflected in the boundary conditions (16a) and (16b). Yet the proposed variational principle involves a relatively shorter interval $r_0 \leq r \leq \infty$, which represents an inconsistency of the present method. However, noting that for heavily doped semiconductors the value of r_0 would be very small (as small as 0.01 \AA), the error resulting from the said inconsistency may be considered to be negligibly small.

III. DISCUSSIONS

A new procedure for the solution of Poisson's equation in the framework of equivalent variational procedure has been discussed. The procedure appears to be far more general than most of the methods available in the literature. It is general enough to be valid for both lightly doped and heavily doped semiconductors.

The greatest strength of the Csavinszky's method lies in the fact that unlike the earlier one,^{11,23} it takes both higher-order terms of the expansion of the second Fermi-Dirac integral of Eq. (2) into account, and considers the effect of spatial variation of the dielectric constant. As noted by Adawi,¹⁰ consideration of higher-order terms of the expansion of this Fermi-Dirac integral is vital to the acceptability of the end result. The accuracy of Csavinszky's method depends largely on the expansion of this second Fermi-Dirac integral of Eq. (2), and on how many terms of the expansion of this Fermi-Dirac integral are taken into consideration. For degenerate semiconductors η varies approximately between 10 to 20, and at room temperature $e_0/kT \approx 0.387 \times 10^2 \text{ V}^{-1}$, indicating that the expansion of $F_{1/2}(\eta + e_0\phi/kT)$ is possible only when $\phi(r)$ is significantly small. It occurs only at large values of r appropriate for lowly doped semiconductors. For heavily doped semiconductors, the screening length becomes small, and consequently the idea of small $\phi(r)$ at large r becomes physically meaningless. This renders Csavinszky's method to be quite unsuitable for heavily doped semiconductors. The potential obtained by the same method is seemingly good enough only for room-temperature as well as high-temperature application, but possibly not for low-temperature applications. Note that at low temperatures η becomes smaller and $e_0\phi/kT$ larger, which obscures Taylor's series-expansion method adopted by Csavinszky. In a separate investigation²² Csavinszky and Morrow attempted to study the small- r behavior of the nonlinear Poisson's equation for the potential of a donor ion in Si and Ge. The method is good for estimating only small- r behavior, but not the large- r behavior, of the Poisson's equation. Further, the method is based on a very crude approximation of the Fermi-

Dirac integral of order $\frac{1}{2}$, which is valid only for a small domain of degeneracy of the semiconductors. Thus the method may provide insignificant information when used to study problems of practical interest. For moderately doped semiconductors, the method remains valid, provided quite larger number of terms of the expansion of this Fermi-Dirac integral are taken into account. However, when this is done, the method becomes extremely cumbersome. When the spatial variation of the dielectric constant is additionally taken into account in the same treatment, the solution becomes practically intractable.

Let us now turn to the present method. This method does not attempt at all to expand the second Fermi-Dirac integral of Eq. (2) using Taylor's series-expansion method. Rather, it makes use of a polynomial approximation Eq. (4b) to express $F_{1/2}(\eta)$ as a function of η . This allows $\rho(r)$ to be expressed in terms of a polynomial of ϕ . As Eq. (4b) appears to be highly accurate for non-degenerate, moderately degenerate, and highly degenerate semiconductors, Eq. (5) is useful for all possible values of $\phi(r)$, and over a wide range of temperatures. Unlike Csavinszky's method, Eq. (4b) allows us to arrive at Eq. (5) regardless of whether η is smaller or larger than $e_0\phi/kT$ due to variation of temperatures. Terms like "small- r behavior" and "large- r behavior" are quite irrelevant in the present method; it is useful practically for "all- r behavior" of the nonlinear Poisson's equation.

In conclusion, a unified approach for the solution of nonlinear Poisson's equation has been proposed. The approach is simple and accurate, and promises to be very widely applicable. It points to the major weaknesses of the earlier methods, and seems to demonstrate novelty and uniqueness in avenues where Csavinszky's method may fail. The information that it attempts to provide to the general readership may have a significantly large impact on the fundamental theoretical analyses of tomorrow's digital and electronic engineering problems.

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