# Large-$r$ form for the potential due to an impurity ion in a medium with spatially variable dielectric constant

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(Received 25 July 1980)

In the linearized theory, Poisson's equation for the potential $\phi(r)$ due to an impurity ion in a semiconductor is $\vec{\nabla}\cdot(K\vec{\nabla}\phi)-K_\infty R_0^{-2}\phi=0$. Here $K(r)$ is the spatially varying dielectric constant, $K_\infty\equiv K(\infty)$ and $R_0$ is the Dingle length. The large-$r$ solution is $\phi\rightarrow Ae_0e^{-r/R_0}/(K_\infty r)$ where $e_0$ is the electronic charge. In this article the value of the constant $A$, which is unity if $K$ is not spatially varying, is investigated. An integral theorem is derived which relates the change $\delta A$ in $A$ to a change $\delta K(r)$ in $K(r)$. This integral theorem employs a "complementary" potential $\tilde{\phi}(r)$ which diverges exponentially at large $r$. It is shown that $\delta A$ is proportional to $(r_0/R_0)^2$ where $r_0$ is the range of the spatially varying part of $K(r)$. Because of this small ratio, the expected value of $A$ is, in typical cases, less than unity by an amount of the order $10^{-2}$ or less. Two related Poisson equations are also discussed.

## INTRODUCTION

Recently there has been considerable interest in the potential due to an (assumed pointlike) impurity ion in a semiconductor. A knowledge of this potential would enable one to calculate the electron scattering due to this impurity ion and therefore to obtain the mobility. An early approach to this problem is that of Dingle[1] which leads to a nonlinear Poisson-type equation for the potential $\phi(r)$. The nonlinearity arises because the screening charge density $\rho$ is a nonlinear function of $\phi$. As an approximation, this screening charge density can be linearized in $\phi$; the solution to this linearized theory being the Dingle potential $\phi_D$:

$$\phi_D=e_0e^{-r/R_0}/(K_\infty r)\,. \tag{1}$$

Here $r$ is the distance from the impurity ion, $R_0$ is a characteristic length called the Dingle length (typically many Bohr radii), $e_0$ is the magnitude of the electron charge, and $K_\infty$ is the static dielectric constant. (In previous articles, this static dielectric constant was denoted by $K_0$; for purposes of the present article, $K_\infty$ is a more suitable notation. Its value is approximately 12 for Si and 16 for Ge.)

An interesting modification of Dingle's theory has recently been proposed by Csavinszky.[2] This modification consists of replacing the (spatially independent) dielectric constant with a spatially varying dielectric constant $K=K(r)$. Retaining the linear approximation of Dingle, Csavinsky obtained the following Poisson equation for the potential $\phi(r)$:

$$\vec{\nabla}\cdot(K\vec{\nabla}\phi)-K_\infty R_0^{-2}\phi=0\,, \tag{2}$$

where $K_\infty\equiv K(r\rightarrow\infty)$. The boundary conditions for $\phi(r)$ are

$$\phi\rightarrow e_0/(K_0r)\ \text{for}\ r\rightarrow 0\,, \tag{3}$$

$$\phi\rightarrow 0\ \text{for}\ r\rightarrow\infty. \tag{4}$$

Here $K_0\equiv K(r\rightarrow 0)$. Equation (3) expresses the fact that there is a single-charged positive ion at the origin. Equation (4) is the usual condition on the potential at large distances. Note that if $K(r)=K_\infty$, one recovers the Dingle solution (1).

For large $r$, $K(r)$ approaches $K_\infty$. The general solution of the Poisson equation (2) for large $r$ is therefore

$$\phi=e_0(Ae^{-r/R_0}+Be^{+r/R_0})/(K_\infty r)\,. \tag{5}$$

Here $A$ and $B$ are constants; the factors of $e_0$ and $K_\infty$ have been inserted for convenience. The boundary condition (4) then implies that $B=0$. Thus the solution for large $r$ must be of the form

$$\phi=Ae_0e^{-r/R_0}/(K_\infty r)\,. \tag{6}$$

If $K(r)=K_\infty$ everywhere (the Dingle case), then the Dingle solution (1) applies and therefore $A=1$. However, if $K$ is spatially varying, then $A$ *need not equal unity*. Several authors, either implicitly or explicitly, have implied that $A$ must be unity; this belief was apparently based on the fact that the differential equation (2) has the same asymptotic (large-$r$) form for variable $K$ as it has for constant $K$. Csavinszky[3] and Richardson and Scarfone[4] both employ a potential [obtained via a variational principle approximately equivalent to (2)] which has $A$ equal to unity. On the other hand, Morrow and Csavinszky[5] and Meyer[6] both report that a numerical solution to (2) yields a potential with $A$ different from unity (in fact, with $A<1$).

In many cases of practical interest, the bulk of the scattering due to this potential arises from the large-$r$ "tail" of $\phi$; therefore the value of $A$ can be of extreme importance in the determination of the electron mobility. The purpose of this article is to investigate the manner in which the value of $A$ changes due to a change in $K(r)$. In particular, we shall investigate how $A$ changes from its value of unity if $K$ changes from $K = K_\infty$ to $K = K(r)$.

The dielectric constant $K(r)$ is spatially varying in the manner shown in Fig. 1. Here $K_0 \equiv K(0)$, $K_\infty \equiv K(\infty)$, and $r_0$ is the "range" of the spatially varying part of the dielectric constant (typically $K_0$ is unity, $K_\infty$ is 12 or 16, and $r_0$ is of the order of a Bohr radius). Also shown in the figure is a slightly varied dielectric constant $K(r) + \delta K(r)$, the variation being such that the asymptotic value $K_\infty$ remains fixed. In the next section, an integral theorem will be derived which relates the change $\delta A$ in $A$ to the change $\delta K(r)$ in $K(r)$.

As for the actual form of the spatially variable dielectric constant $K(r)$, several authors have used the spatial dielectric function $\epsilon(r)$ based on the Penn model. Recently, Csavinszky[7] has pointed out that the dielectric constant $K(r)$ should not be identified directly with the dielectric function $\epsilon(r)$. This reference shows the correct relation between these to be

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

where the prime denotes $d/dr$.

## INTEGRAL THEOREM FOR THE POISSON EQUATION

The potential $\phi(r)$ obeys the differential equation

$$\vec{\nabla}\cdot(K\vec{\nabla}\phi) - K_\infty R_0^{-2}\phi = 0. \tag{7}$$

The small- and large-$r$ asymptotic forms for $\phi(r)$ are

$$\phi \to (e_0/K_0)[r^{-1} + a + br + \cdots + \ln(r)(\alpha + \beta r + \cdots)] \quad \text{for } r \to 0, \tag{8}$$

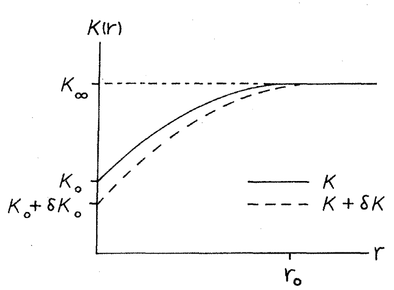


FIG. 1. Spatially varying dielectric constant $K(r)$ as a function of $r$. Typical values are $K_\infty = 12$ for Si (16 for Ge) and $K_0 = 1$. The range $r_0$ of the spatially varying part of $K(r)$ is of the order of one Bohr radius. Also shown is a slightly varied dielectric constant $K(r) + \delta K(r)$, the variation being such as to preserve the asymptotic value $K_\infty$.

$$\phi \to A\, e_0 e^{-r/R_0}/(K_\infty r) \quad \text{for } r \to \infty. \tag{9}$$

These are consistent with Eqs. (3) and (4); the ln terms are needed according to the behavior of $K(r)$ near $r = 0$.

The integral theorem to be derived below makes use of a "complementary" potential $\tilde{\phi}(r)$ which also satisfies the same differential equation as $\phi$, namely,

$$\vec{\nabla}\cdot(K\vec{\nabla}\tilde{\phi}) - K_\infty R_0^{-2}\tilde{\phi} = 0. \tag{10}$$

The small-$r$ form for $\tilde{\phi}$ is taken to be similar to that for $\phi$

$$\tilde{\phi} \to (e_0/K_0)[r^{-1} + \tilde{a} + \tilde{b}r + \cdots + \ln(r)(\tilde{\alpha} + \tilde{\beta}r + \cdots)] \quad \text{for } r \to 0. \tag{11}$$

However, the large-$r$ form for $\tilde{\phi}$ is taken to be complementary to that for $\phi$ in the sense that

$$\tilde{\phi} \to \tilde{A}e_0 e^{+r/R_0}/(K_\infty r) + (\text{zero})e^{-r/R_0}/(K_\infty r) \quad \text{for } r \to \infty. \tag{12}$$

Here it is understood that for large $r$, $\tilde{\phi}$ involves only an increasing exponential function and no decreasing exponential function. Thus both $\phi$ and $\tilde{\phi}$ satisfy the same differential equation (2) and obey the same boundary condition (3) for $r \to 0$; they differ in their behavior for $r \to \infty$ in that $\phi$ involves a purely decreasing exponential function of $r$ while $\tilde{\phi}$ involves a purely increasing function of $r$.

Corresponding to the Dingle solution (1), one has the complementary Dingle solution for the case $K = K_\infty$:

$$\tilde{\phi}_D = e_0 e^{+r/R_0}/K_\infty r. \tag{13}$$

Note that $A = 1$ for the Dingle solution and that $\tilde{A} = 1$ for the complementary Dingle solution.

The general solution of Eq. (7) for large $r$ consists of a linear combination of an increasing and a decreasing exponential function of $r$ (divided by $r$). Substitution of the small-$r$ form (8) into (7) shows that the leading coefficient $a$ is arbitrary; in fact, it is the selection of the correct value for $a$ which ensures that the large-$r$ boundary condition (9) for $\phi$ will be satisfied. Similarly, the selection of the correct value for $\tilde{a}$ in (11) ensures that the large-$r$ boundary condition (12) will be satisfied for $\tilde{\phi}$. As for the leading coefficient in the logarithmic part of the potential, direct substitution of the small-$r$ form [(8) or (11)] into the differential equation [(7) or (10)] shows that

$$\tilde{\alpha} = \alpha, \tag{14}$$

their common value being $K'(0)/K(0)$ where the prime denotes $d/dr$.

Let $f(r)$ and $g(r)$ be any two solutions of the

Poisson equation (7):

$$\vec{\nabla}\cdot(K\vec{\nabla}f)-K_\infty R_0^{-2}f=0\,, \tag{15}$$

$$\vec{\nabla}\cdot(K\vec{\nabla}g)-K_\infty R_0^{-2}g=0\,. \tag{16}$$

Multiplying (15) by $g$ and (16) by $f$ and then subtracting gives

$$\vec{\nabla}\cdot(fK\vec{\nabla}g-gK\vec{\nabla}f)=0\,. \tag{17}$$

Next, Eq. (17) is integrated over the annular volume between the spherical surfaces $r=\epsilon$ and $r=R$. Letting $d\tau$ be the volume element, this integration will be denoted as follows:

$$\int_\epsilon^R \vec{\nabla}\cdot(fK\vec{\nabla}g-gK\vec{\nabla}f)\,d\tau=0\,. \tag{18}$$

Application of Gauss's theorem to this volume integral of a divergence gives

$$+4\pi R^2\left(fK\frac{dg}{dr}-gK\frac{df}{dr}\right)\bigg|_{r=R} -4\pi\epsilon^2\left(fK\frac{dg}{dr}-gK\frac{df}{dr}\right)\bigg|_{r=\epsilon}=0. \tag{19}$$

We now choose $f=\phi$ and $g=\tilde{\phi}$ [note that both of these satisfy the Poisson equation (7)] and take the limit in (19) as $\epsilon\to 0$ and $R\to\infty$. Substituting the large- and small-$r$ forms (8), (9), (11), and (12) into (19) and making use of (14), one finds that

$$\tilde{a}-a=2\frac{K_0}{K_\infty}\frac{A\tilde{A}}{R_0}\,. \tag{20}$$

This relation will be used later [to process Eq. (28)]. As a check, we note that Eq. (20) is satisfied in the Dingle case ($K_0=K_\infty$, $a=-1/R_0$, $\tilde{a}=+1/R_0$, $A=\tilde{A}=1$).

Again, let $f(r)$ and $g(r)$ be any two solutions of the Poisson equation (7) so that Eqs. (15) and (16) apply. Multiplying (16) by $f$ and integrating over the annular volume from $r=\epsilon$ to $r=R$, we have

$$\int_\epsilon^R f[\vec{\nabla}\cdot(K\vec{\nabla}g)-K_\infty R_0^{-2}g]\,d\tau=0\,. \tag{21}$$

Now take the variation $\delta$ associated with a variation $\delta K(r)$ in $K(r)$, this variation in $K(r)$ being such as to preserve the asymptotic value $K_\infty$ of $K(r)$, i.e., $\delta K(\infty)=0$. Thus $K(r)\to K(r)+\delta K(r)$, $f(r)\to f(r)+\delta f(r)$, and $g(r)\to g(r)+\delta g(r)$. In view of (16), the $\delta$ variation of Eq. (21) becomes

$$\int f\{\vec{\nabla}\cdot[K\vec{\nabla}(\delta g)]-K_\infty R_0^{-2}\delta g\}\,d\tau + \int f\,\vec{\nabla}\cdot(\delta K\,\vec{\nabla}g)d\tau=0\,. \tag{22}$$

Using the identities

$$f\vec{\nabla}\cdot[K\vec{\nabla}(\delta g)]=\vec{\nabla}\cdot[fK\vec{\nabla}(\delta g)-(\delta g)K\vec{\nabla}f] +(\delta g)\vec{\nabla}\cdot(K\vec{\nabla}f)\,, \tag{23}$$

$$f\vec{\nabla}\cdot(\delta K\,\vec{\nabla}g)=\vec{\nabla}\cdot[(\delta K)f\,\vec{\nabla}g]-(\delta K)\,\vec{\nabla}f\cdot\vec{\nabla}g\,, \tag{24}$$

and Eq. (15), Eq. (22) can be written

$$\int\vec{\nabla}\cdot[fK\vec{\nabla}(\delta g)-(\delta g)K\vec{\nabla}f]\,d\tau + \int\vec{\nabla}\cdot[(\delta K)f\,\vec{\nabla}g]d\tau-\int(\delta K)\vec{\nabla}f\cdot\vec{\nabla}g\,d\tau=0\,. \tag{25}$$

We now choose $f=\phi$ and $g=\tilde{\phi}-\phi$ [note that both of these satisfy the Poisson equation (7)]. We shall be interested in the limit $\epsilon\to 0$, $R\to\infty$; the large- and small-$r$ forms for $\phi$ and $\tilde{\phi}$ are given in Eqs. (8), (9), (11), and (12). As for the large- and small-$r$ forms for $\delta g=\delta(\tilde{\phi}-\phi)$, we have

$$\begin{aligned}\delta g\to{}&(e_0/K_0)[\delta(\tilde{a}-a)+\cdots+r\ln(r)\delta(\tilde{\beta}-\beta)+\cdots]\\ &-(e_0\delta K_0/K_0^2)[(\tilde{a}-a)+\cdots+r\ln(r)(\tilde{\beta}-\beta)+\cdots]\\ &\text{for } r\to 0\,,\end{aligned} \tag{26}$$

$$\delta g\to(\delta\tilde{A})e_0e^{+r/R_0}/(K_\infty r)-(\delta A)e_0e^{-r/R_0}/(K_\infty r) \quad \text{for } r\to\infty. \tag{27}$$

Here the terms involving $\alpha$ and $\tilde{\alpha}$ cancel in view of (14). Note that the variation $\delta K_0$ in $K_0$ is taken into consideration; the variation in $K_\infty$, however, is omitted due to the stated assumption that $\delta K(\infty)=0$.

In Eq. (25), we convert the two divergence volume integrals into surface integrals, substitute the large- and small-$r$ forms for $f, g$, and $\delta g$, and take the limit $\epsilon\to 0$, $R\to\infty$. After some algebra we find

$$\begin{aligned}&(4\pi_0^2/K_\infty)(2A\,\delta\tilde{A}/R_0)\\ &\quad-(4\pi e_0^2/K_0)[\delta(\tilde{a}-a)-(\tilde{a}-a)\,\delta K_0/K_0]\\ &\quad-\int(\delta K)\vec{\nabla}\phi\cdot\vec{\nabla}(\tilde{\phi}-\phi)\,d\tau=0\,.\end{aligned} \tag{28}$$

Taking the $\delta$ variation of Eq. (20),

$$\begin{aligned}\delta(\tilde{a}-a)&=2A\tilde{A}\delta K_0/(K_\infty R_0)\\ &\quad+2K_0(A\delta\tilde{A}+\tilde{A}\,\delta A)/(K_\infty R_0)\\ &=(\tilde{a}-a)\,\delta K_0/K_0+2K_0(A\,\delta\tilde{A}+\tilde{A}\,\delta A)/(K_\infty R_0)\,,\end{aligned} \tag{29}$$

where the last form is obtained using (20) again.

Next, Eq. (29) is used to eliminate $\delta(\tilde{a}-a)$ in Eq. (28). The terms involving $\delta K_0$ cancel, the final result being

$$\delta A = -K_\infty R_0/(8\pi e_0^2 \tilde{A}) \int_{\text{all space}} \delta K\, \vec{\nabla}\phi \cdot \vec{\nabla}(\tilde{\phi}-\phi)\, d\tau. \tag{30}$$

Equation (30) is the desired integral theorem. It gives the change $\delta A$ in $A$ in terms of the change $\delta K(r)$ in $K(r)$.

It can be shown (see Appendix A) that the total coefficient of $\delta K$ in Eq. (30) is positive. We may imagine starting with the Dingle case [$A = 1$, $K(r) = K_\infty$] and then changing $K(r)$ into its actual form (as shown in Fig. 1) by means of successive changes with $\delta K(r) < 0$. It then follows that for each of these changes, $\delta A < 0$. Because of all these negative changes of $A$, the final value of $A$ must be less that its value for the Dingle case, i.e.,

$$A < 1. \tag{31}$$

This constitutes one of the major results of this article: The tail of the potential associated with the spatially varying dielectric constant is *smaller* than that associated with the Dingle potential.

To obtain an estimate of the actual value of $A$, we shall apply the "Dingle approximation" to Eq. (30). Thus we take $\tilde{A} = 1$, $K_0 = K_\infty$, $\phi = \phi_D$, and $\tilde{\phi} = \tilde{\phi}_D$. If we make the further approximation that $\delta K(r)$ is of short range, in particular that

$$\delta K(r) = \begin{cases} \delta K = \text{const} \quad \text{for } 0 \le r \le r_0 & \text{(32a)} \\ 0 \quad \text{for } r_0 < r, & \text{(32b)} \end{cases}$$

with

$$r_0 \ll R_0, \tag{33}$$

then

$$\phi \simeq e_0/(K_\infty r)[1 - r/R_0 + r^2/(2R_0^2) - r^3/(6R_0^3) + \cdots], \tag{34a}$$

$$\tilde{\phi} \simeq e_0/(K_\infty r)[1 + r/R_0 + r^2/(2R_0^2) + r^3/(6R_0^3) + \cdots]. \tag{34b}$$

Substituting these into (30) and retaining only the leading terms in $r/R_0$ gives

$$\delta A \simeq -R_0 \frac{\delta K}{8\pi K_\infty} \int_0^{r_0} (-1/r^2)[2r/(3R_0^3)]\, 4\pi r^2\, dr,$$

or

$$\delta A \simeq \frac{1}{6} \frac{\delta K}{K_\infty} \left(\frac{r_0}{R_0}\right)^2. \tag{35}$$

This is the other major result of this article: The change $\delta A$ in $A$ associated with the change $\delta K$ in $K(r)$ is of the order $(r_0/R_0)^2$. Here $r_0$ is the range of the variation in $K(r)$ and $R_0$ is the Dingle length.

If we take the liberty of applying Eq. (35) to a finite $\delta K$, then typical data might be the following: $-\delta K = K_\infty - K_0 = 12 - 1$ to $16 - 1$, $r_0/R_0 = 10^{-1}$ to $10^{-2}$. This gives, as the estimate for the change in $A$,

$$\delta A \simeq -10^{-3} \text{ to } -10^{-5}. \tag{36}$$

Thus, although $A$ is not equal to unity, its departure from unity can be expected to be *very small* in many practical cases.

In obtaining the estimate (35), three assumptions were made: (i) that $\phi$ and $\tilde{\phi}$ could be replaced by their corresponding Dingle potentials $\phi_D$ and $\tilde{\phi}_D$, respectively, (ii) that $\delta K$ was infinitessimal, and (iii) that $r_0 \ll R_0$. In the next section it is shown that an analog of (35) exists provided only that assumption (iii) concerning the short range of $\delta K$ is satisfied.

## SHORT-RANGE APPROXIMATION

Suppose that the range $r_0$ of $\delta K(r)$ is short; in practice this would be satisfied by $r_0 \ll R_0$. Then, as will be shown below, Eq. (30) can be processed into a form which allows one to integrate with respect to $\delta K$. This will lead to an expression for the *finite* change $\Delta A$ in $A$ associated with the *finite* change $\Delta K(r)$ in $K(r)$. We shall assume that $\Delta K$ is built up from a succession of $\delta K$'s of the form (32), i.e., that $\Delta K(r)$ is a "square well."

We start with the fact that $\tilde{\phi} - \phi$ satisfies the Poisson equation

$$\vec{\nabla} \cdot \{K \vec{\nabla}(\tilde{\phi} - \phi)\} - K_\infty R_0^{-2}(\tilde{\phi} - \phi) = 0. \tag{37}$$

Next, this is integrated $\int_\epsilon^r \{\ \}\, d\tau$ with the limit $\epsilon \to 0$ understood and with $r \le r_0$. The first term can be converted to a surface integral; the contribution at the inner surface ($r = \epsilon$) vanishes in the limit $\epsilon \to 0$ due to the fact that $\tilde{\phi} - \phi$ is finite at the origin. The second term can be evaluated by using the short-range approximation $\tilde{\phi} - \phi = (e_0/K_0)(\tilde{a} - a + \cdots)$. This gives, with the aid of (20),

$$\frac{d}{dr}(\tilde{\phi} - \phi) \simeq \frac{2e_0 A \tilde{A} r}{3KR_0^3}, \quad r \le r_0. \tag{38}$$

Substituting (38) into (30) and using the short-range approximation $d\phi/dr \simeq (e_0/K_0)(r^{-1} + \cdots)$, one obtains

$$\delta A = \frac{1}{6} \frac{K_\infty A \delta K}{K_0^2} \left(\frac{r_0}{R_0}\right)^2. \tag{39}$$

This is the generalization of Eq. (35) and reduces to it in the Dingle case ($K_0 \simeq K_\infty$, $A = 1$). However, note that Eq. (39) applies to the perturbation of *any* $K(r)$, not just the Dingle case. It is quite fortuitous that, in substituting (38) into (30), the factor $\tilde{A}$ cancels out; this will enable us to integrate (39) with respect to $\delta K$. To do this, note that starting with the Dingle case; $A$ varies from 1 to $1+\Delta A$, $K_0$ varies from $K_\infty$ to $K_\infty + \Delta K$, $K_\infty$ remains fixed, and [from (32)] $\delta K = \delta K_0$. From (39) we have

$$\int \frac{dA}{A} = \tfrac{1}{6} K_\infty \left(\frac{r_0}{R_0}\right)^2 \int \frac{dK_0}{K_0^2} .$$

Hence the desired analog of Eq. (35 is

$$\ln(1+\Delta A) = \frac{1}{6}\left(1 - \frac{K_\infty}{K_\infty + \Delta K}\right)\left(\frac{r_0}{R_0}\right)^2 . \tag{40}$$

Assuming that both the short-range approximation and the "square-well" form (32) for $\Delta K$ apply, Eq. (40) is an *exact* expression for the *finite* change $\Delta A$ associated with the *finite* change $\Delta K$. When typical numbers [such as those used to obtain the estimate (36)] are substituted into (40), it is found that $\Delta A$ is larger than the estimate (36) by about one order of magnitude. Thus there is still every reason to believe that the departure of $A$ from unity will be small. The principle reason for this smallness is the proportionality

$$\delta A \propto (r_0/R_0)^2 \tag{41}$$

on the square of the ratio of the two naturally occuring lengths.

The proportionality (41) agrees with a result of Morrow[8] obtained by approximately solving an integral equation equivalent to the Poisson differential equation. [See Eq. (16) of Ref. 8. Morrow's $r_d$ corresponds to the present $r_0$ and his $R_D$ corresponds to the present $R_0$.]

## INTEGRAL THEOREMS FOR RELATED POISSON EQUATIONS

In Csavinszky's original work on Poisson's equation incorporating spatially varying dielectric constants,[2] two facets which are present in the correct formulation were, for expediency, ignored: (i) the term involving $\vec{\nabla} K$ in (2) was omitted and (ii) the boundary condition at the origin involved $K_\infty$ (the Dingle case boundary condition) instead of $K_0$ in (3). Thus the problem discussed in this reference was (in the present notation)

$$\nabla^2\phi - K_\infty R_0^{-2}\,\phi/K = 0, \tag{42a}$$

$$\phi \to e_0/K_\infty r \quad \text{for } r \to 0, \tag{42b}$$

$$\phi \to A e_0 e^{-r/R_0}/K_\infty r \quad \text{for } r \to \infty . \tag{42c}$$

This differential equation can be treated in a manner quite similar to that used in the preceding section: A complementary potential $\tilde{\phi}$ is defined such that it obeys Eqs. (42) except that the sign of the exponent in (42c) is positive and $A$ is replaced by $\tilde{A}$. Since the calculation is so similar to that of the preceding section, details will not be presented. The terms involving $\delta K_0$ are, in this case, entirely absent (whereas in the preceding section these terms cancelled). The final result [the analog of Eq. (30)] is

$$\delta A = \frac{K_0 K_\infty^2}{8\pi e_0^2 R_0 \tilde{A}} \int_{\text{all space}} \phi(\tilde{\phi} - \phi)\,\frac{\delta K}{K^2}\,d\tau . \tag{43}$$

Again, it can be shown (see Appendix B) that the total coefficient of $\delta K$ in Eq. (43) is positive. Therefore, by the same argument used in the preceding section, it follows that

$$A < 1 \tag{44}$$

for Eqs. (42) with a $K(r)$ as shown in Fig. 1.

To obtain an estimate of the actual value of $A$, we shall apply the "Dingle approximation" to Eq. (43). Thus we take $\tilde{A} = 1$, $K_0 = K_\infty$, $\phi = \phi_D$, and $\tilde{\phi} = \tilde{\phi}_D$. If we make the further approximation that $\delta K(r)$ is of short range, in particular that Eqs. (32)–(34) apply, then Eq. (43) gives

$$\delta A \simeq \frac{1}{2}\,\frac{\delta K}{K_\infty}\left(\frac{r_0}{R_0}\right)^2 . \tag{45}$$

This is qualitatively similar to its analog, Eq. (35), but is larger by a factor of 3. Thus, again we obtain the proportionality

$$\delta A \propto \left(\frac{r_0}{R_0}\right)^2 , \tag{46}$$

and we may therefore expect the value of $\delta A$ to be very small.

One final Poisson equation is obtained by neglecting the $\vec{\nabla} K$ term while restoring the correct boundary condition at $r \to 0$. This equation was discussed by Csavinszky[3] and by Richardson and Scarfone.[4] In the present notation, this problem is

$$\nabla^2\phi - K_\infty R_0^{-2}\,\phi/K = 0, \tag{47a}$$

$$\phi \to e_0/K_0 r \quad \text{for } r \to 0, \tag{47b}$$

$$\phi \to A e_0 e^{-r/R_0}/K_\infty r \quad \text{for } r \to \infty . \tag{47c}$$

This is the same as Eqs. (42) except that (47b) has the factor $K_0$ in the denominator where (42b) had the factor $K_\infty$. Proceeding as before, an integral theorem can be derived for $\delta A$. In this case the terms involving $\delta K_0$ do not cancel out. The result is

$$\delta A = \frac{K_\infty^3}{8\pi e_0^2 R_0 \tilde{A}} \int_{\text{all space}} \phi(\tilde{\phi} - \phi)\,d\tau - A\,\frac{\delta K_0}{K_0} . \tag{48}$$

The first (integral) term is similar to Eq. (43) except for an additional factor of $K_\infty/K_0$. Thus it would, in the Dingle and short-range approximations, contribute a small quantity proportional to $(r_0/R_0)^2$. The last term in (48), however, can be expected to contribute a large quantity which is independent of the range $r_0$. Neglecting the small integral term, the remainder of Eq. (48) can be integrated with respect to $K_0$ to yield

$$A = K_\infty / K_0 . \tag{49}$$

This shows that the value of $A$ can be expected to change from unity to about 12 or 16 in typical cases.

## DISCUSSION

Poisson's equation for the potential $\phi(r)$ associated with an impurity ion in a semiconductor is

$$\vec{\nabla}\cdot(K\vec{\nabla}\phi) - K_\infty R_0^{-2}\phi = 0, \tag{50a}$$

with the boundary conditions

$$\phi \to e_0/K_0 r \quad \text{for } r\to 0, \tag{50b}$$

$$\phi \to 0 \quad \text{for } r \to \infty. \tag{50c}$$

Here $K(r)$ is the spatially varying dielectric constant, $K_0 \equiv K(0)$ and $K_\infty \equiv K(\infty)$. The large-$r$ form for $\phi$ is

$$\phi \to A e_0 e^{-r/R_0}/K_\infty r . \tag{51}$$

In the "Dingle case," i.e., $K(r)$ = constant, the value of $A$ is unity. If $K(r)$ is not constant, then $A$ need not be unity. In this article the dependence of the factor $A$ upon changes in the function $K(r)$ was investigated. Several integral theorems were derived which gave the change $\Delta A$ in $A$ due to a change $\Delta K$ in $K$ for both the above Poisson equation and two related Poisson equations. These integral theorems made use of a complementary potential $\bar{\phi}$ which diverged exponentially for large $r$.

For the Poisson equation (50), the major results were that for a $K(r)$ such as shown in Fig. 1: (i) $A$ is less than unity; (ii) $\Delta A$ is proportional to $(r_0/R_0)^2$, where $r_0$ is the range of the varying part of $K(r)$ and it is assumed that $r_0 \ll R_0$. Typical numerical values indicate that $\Delta A$ should be less than approximately $10^{-2}$.

A related Poisson equation which was studied is similar to (50) except that the $\vec{\nabla}K$ term is neglected and an incorrect boundary condition for $r\to 0$ [namely, the replacement of $K_0$ with $K_\infty$ in (50b)] is used. It is found that these two omissions almost cancel out in the sense that the above results [(i) and (ii)] are still true although the exact expression for $\Delta K$ is now larger by a factor of 3.

Another related Poisson equation neglects the $\vec{\nabla}K$ term but restores the correct boundary condition (50b). In this case the change $\Delta A$ in $A$ turns out to be very large, the predicted value for $A$ being more than 10.

In conclusion, if the correct Poisson equation (50) is used, the expected value of $A$ should be smaller than unity but by an amount $\Delta A$ which is so small as to render this change in $A$ to be negligible in many practical cases. However, since this smallness was due to the factor $(r_0/R_0)^2$, this effect would become important if the Dingle radius $R_0$ were comparable to the range $r_0$ of the spatially varying part of the dielectric constant $K(r)$.

## APPENDIX A

We seek to show that the total coefficient of $\delta K$ in Eq. (30) is positive. The proof consists of two parts: (a) that $d\phi/dr < 0$ and (b) that $(1/\bar{A})d(\bar{\phi} - \phi)/dr > 0$. These two facts, combined with the negative sign in (30), assure the desired result.

(a) To show that $d\phi/dr < 0$ for all $r$. Clearly this is true for $r\to 0$. By continuity, if $d\phi/dr > 0$ somewhere, there would exist a certain $r = r_1$ at which $d\phi/dr = 0$. Multiplying the Poisson equation (7) for $\phi$ by $\phi$ and integrating over the annular volume from $r = r_1$ to $r = \infty$,

$$\int_{r_1}^{\infty} \phi[\vec{\nabla}\cdot(K\vec{\nabla}\phi) - K_\infty R_0^{-2}\phi]\,d\tau = 0. \tag{A1}$$

This can be rearranged to give

$$\int_{r_1}^{\infty} \vec{\nabla}\cdot(\phi K\vec{\nabla}\phi)\,d\tau = \int_{r_1}^{\infty} K\vec{\nabla}\phi\cdot\vec{\nabla}\phi\,d\tau + K_\infty R_0^{-2}\int_{r_1}^{\infty}\phi^2\,d\tau . \tag{A2}$$

Both terms on the right-hand side of (A2) are manifestly positive. Transforming the left-hand side to a surface integral yields

$$4\pi r^2\phi K\frac{d\phi}{dr}\bigg|_{r\to\infty} - 4\pi r^2\phi K\frac{d\phi}{dr}\bigg|_{r=r_1} > 0 . \tag{A3}$$

This is a contradiction since both terms on the left-hand side are zero.

(b) To show that $(1/\bar{A})d(\bar{\phi} - \phi)/dr > 0$ for all $r$. Clearly this is true for $r\to\infty$. By continuity, if $(1/\bar{A})d(\bar{\phi} - \phi)/dr < 0$ somewhere, there would exist a certain $r = r_2$ at which $d(\bar{\phi} - \phi)/dr = 0$. Multiplying the Poisson equation (7) for $(\bar{\phi} - \phi)$ by $(\bar{\phi} - \phi)$ and integrating over the annular volume from $r = 0$ to $r = r_2$,

$$\int_0^{r_2} (\bar{\phi} - \phi)\{\vec{\nabla}\cdot[K\vec{\nabla}(\bar{\phi} - \phi)] - K_\infty R_0^{-2}(\bar{\phi} - \phi)\}\,d\tau = 0 . \tag{A4}$$

This can be rearranged to give

$$\int_0^{r_2} \vec{\nabla}\cdot[(\tilde{\phi}-\phi)K\vec{\nabla}(\tilde{\phi}-\phi)]\,d\tau = \int_0^{r_2} K\vec{\nabla}(\tilde{\phi}-\phi)\cdot\vec{\nabla}(\tilde{\phi}-\phi)\,d\tau + K_\infty R_0^{-2}\int_0^{r_2}(\tilde{\phi}-\phi)^2\,d\tau\,. \quad \text{(A5)}$$

Both terms on the right-hand side of (A5) are manifestly positive. Transforming the left-hand side to a surface integral yields

$$4\pi r^2(\tilde{\phi}-\phi)\left.\frac{d(\tilde{\phi}-\phi)}{dr}\right|_{r=r_2} - 4\pi r^2(\tilde{\phi}-\phi)\left.\frac{d(\tilde{\phi}-\phi)}{dr}\right|_{r\to 0} > 0\,. \quad \text{(A6)}$$

This is a contradiction since both terms on the left-hand side are zero.

## APPENDIX B

We seek to show that the total coefficient of $\delta K$ in Eq. (43) is positive. The proof consists of two parts: (a) that $\phi > 0$, and (b) that $(1/\tilde{A})(\tilde{\phi}-\phi) > 0$. These two facts assure the desired result.

(a) To show that $\phi > 0$ for all $r$. Clearly this is true for $r \to 0$. By continuity, if $\phi < 0$ somewhere, then there would exist a certain $r = r_1$ at which $\phi = 0$. Multiplying the Poisson equation (42a) for $\phi$ by $\phi$ and integrating over the annular volume from $r = r_1$ to $r = \infty$,

$$\int_{r_1}^{\infty} \phi\left(\nabla^2\phi - \frac{K_\infty R_0^{-2}\phi}{K}\right)d\tau = 0\,. \quad \text{(B1)}$$

This can be rearranged to give

$$\int_{r_1}^{\infty} \vec{\nabla}\cdot(\phi\vec{\nabla}\phi)\,d\tau = \int_{r_1}^{\infty} \vec{\nabla}\phi\cdot\vec{\nabla}\phi\,d\tau + K_\infty R_0^{-2}\int_{r_1}^{\infty}\frac{\phi^2}{K}\,d\tau\,. \quad \text{(B2)}$$

Both terms on the right-hand side of (B2) are manifestly positive. Transforming the left-hand side to a surface integral yields

$$4\pi r^2\phi\left.\frac{d\phi}{dr}\right|_{r\to\infty} - 4\pi r^2\phi\left.\frac{d\phi}{dr}\right|_{r=r_1} > 0\,. \quad \text{(B3)}$$

This is a contradiction since both terms on the left-hand side are zero.

(b) To show that $(1/\tilde{A})(\tilde{\phi}-\phi) > 0$ for all $r$. Clearly this is true for $r \to \infty$. By continuity, if $(1/\tilde{A})(\tilde{\phi}-\phi) < 0$ somewhere, there would exist a certain $r = r_2$ at which $(\tilde{\phi}-\phi) = 0$. Multiplying the Poisson equation (42a) for $(\tilde{\phi}-\phi)$ by $(\tilde{\phi}-\phi)$ and integrating over the annular volume from $r = 0$ to $r = r_2$.

$$\int_0^{r_2}(\tilde{\phi}-\phi)[\nabla^2(\tilde{\phi}-\phi) - K_\infty R_0^{-2}(\tilde{\phi}-\phi)/K]\,d\tau = 0\,. \quad \text{(B4)}$$

This can be rearranged to give

$$\int_0^{r_2}\vec{\nabla}\cdot[(\tilde{\phi}-\phi)]\vec{\nabla}(\tilde{\phi}-\phi)]\,d\tau = \int_0^{r_2}\vec{\nabla}(\tilde{\phi}-\phi)\cdot\vec{\nabla}(\tilde{\phi}-\phi)\,d\tau + K_\infty R_0^{-2}\int_0^{r_2}[(\tilde{\phi}-\phi)^2/K]\,d\tau = 0\,. \quad \text{(B5)}$$

Both terms on the right-hand side are manifestly positive. Transforming the left-hand side to a surface integral yields

$$4\pi r^2(\tilde{\phi}-\phi)\left.\frac{d(\tilde{\phi}-\phi)}{dr}\right|_{r=r_2} - 4\pi r^2(\tilde{\phi}-\phi)\left.\frac{d(\tilde{\phi}-\phi)}{dr}\right|_{r\to 0} > 0\,. \quad \text{(B6)}$$

This is a contradiction since both terms on the left-hand side are zero.

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