Reply to "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"

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The adequacy of our physically based boundary condition is discussed relative to the theoretical boundary condition used by Csavinszky and Morrow. The impurity-ion potentials resulting from the two calculations are compared and contrasted on the basis of their physical behavior and that of the ionized-impurity-limited mobilities to be derived from each.

An equivalent variational principle[1] and the methods of numerical analysis[2] have been used in obtaining approximate solutions of the linearized version of a generalized Poisson's equation for the potential $\phi(r)$ of a pointlike impurity ion in a doped semiconductor medium characterized by a spatially-variable dielectric constant $\kappa(r)$. These treatments are concerned with the development of impurity-ion potentials that embody a more accurate description of dispersive valence screening than that found in the early Dingle theory[3] which yields an exponentially screened Coulomb potential scaled by the inverse of the static dielectric constant κ_0 of the medium.

Various approximate analytic potentials employed as trial functions in the variational technique or as fitting functions in the numerical approach have been used in a number of Born-approximation[4] and partial-wave-theory[5] calculations of ionized-impurity-limited mobility and other quantities related to ionized-impurity scattering in uncompensated semiconductors. These applications of the generalized Dingle theory are deficient in one or more of the following respects:

(1) Usage of the linearized Poisson's equation rather than the complete nonlinearized version.

(2) The potentials are derived from the linearized Poisson's equation with the neglect of a term involving $\kappa'(r)$, where the prime denotes the derivative with respect to r.

(3) One of these potentials incorporates an incorrect boundary condition at small r.

(4) No distinction is made between $\kappa(r)$ and the spatial dielectric function $\epsilon(r)$ of the medium.

(5) Derivations of the potentials imply, either implicitly or explicitly, that the solutions to the linearized Poisson's equation reduce to the Dingle potential $\phi_0(r)$ at sufficiently large r such that $\kappa(r) \to \kappa_0$.

Recent developments by Csavinszky and Morrow (CM) (Ref. 6) correct for the difference between $\kappa(r)$ and $\epsilon(r)$, and explore the large-r behavior $\phi \to A\phi_0$ of the generalized potential, where A is a numerical factor to be determined. (Some theoretical basis for expecting that A will be different from unity has recently been proposed by Brownstein.[7]) CM have obtained approximate solutions to the linearized equation both by an equivalent variational principle and by numerical methods. Obviously, the potential calculated by CM will differ from that calculated by us (SR) because of this distinction between $\kappa(r)$ and $\epsilon(r)$. Furthermore, our form for $\epsilon(r)$ is due to Resta[8] while that used by CM was formulated by Azuma and Shindo.[9] We believe that Resta's dielectric function is physically more reasonable than the Azuma-Shindo function. The former rises smoothly up to a constant value κ_0 and then is defined as constant thereafter. (For example, in the case of silicon the dielectric function is exactly equal to the static dielectric constant κ_0 for r greater than 4.28 a.u.) As we mentioned in our paper, the Azuma-Shindo function is suspect since it rises to a nearly constant value at a larger value of r than was predicted by Srinivasan.[10] Thus, due to these dissimilarities, the actual linearized Poisson's equations solved by SR and by CM are different and should not be expected to yield identical solutions for ϕ.

CM have raised an objection to our use of the boundary condition that $\phi = \phi_0$ for $r = 25$ a.u. in our numerical solution. Such an objection is really a criticism of the common practice in the early calculations of identifying ϕ with ϕ_0 for large r (fifth point listed above). This relationship has a strong intuitive basis and was considered to be additional information characterizing ϕ, rather than a contradiction of the boundary condition at infinity, $\phi \to 0$. The spatial dielectric

function attains its full objective within a relatively short distance and asymptotes to κ_0 at $r=\infty$. Therefore, it would appear reasonable from continuity that $\phi \to \phi_0$ for large r. The theoretical results of Brownstein that $\phi \to A\phi_0$, as previously mentioned, might seem to contradict this assumption. Nevertheless, as stated by Brownstein, for most practical purposes this departure from unity is negligible. Another indication of the closeness of A to unity can be seen in Fig. 1 of Meyer's paper which compares the numerical solution to the generalized linearized Poisson's equation with ϕ_0. In his solution Meyer used the boundary condition, $\phi \to 0$ at infinity. There, it is seen that ϕ/ϕ_0 is essentially indistinguishable from unity for $r>7$ a.u.. In SR, the closeness of A to unity is used as an approximation in the implementation of the numerical boundary condition at infinity. Our choice of "infinity" at 25 a.u. was a compromise between accuracy and computer time. We found very little variation in the results for larger values of "infinity." In this regard, it would be of interest to know the choice of "infinity" used by CM and Meyer in their numerical solution routines.

The potential derived by CM, in contrast to those derived by SR and by Meyer, shows a value for A that is significantly different from unity. For their potential, the behavior of A (defined as "q" by CM) as a function of R_0, the Dingle screening length, is as follows. We see from CM's Fig. 3 that, for small values of R_0, A is small, being as low as 0.7. For large R_0, the value of A asymptotes to some larger value that would appear from this figure to be approximately 0.97. (It is hard to decipher the exact behavior as CM do not carry their solution out to very large values of R_0.) We find such small values of A (i.e., significantly less than unity) in the low-R_0 region to be disconcerting for the following reasons.

(1) When A is less than unity, this indicates that the derived potential is smaller (weaker) than the standard Dingle potential. The effect of the inclusion of the spatial variation of the dielectric function is such that the ion is less screened than with a constant dielectric function. Thus, it would seem plausible that the potential derived from such considerations should be stronger (not weaker) than the Dingle potential.

(2) The further effect of such a "weakened" impurity-ion potential will be to increase the value that would be calculated for ionized-impurity-limited mobility. This trend is away from the experimental points which are usually found to be lower than the traditional (Brooks-Herring) predictions for mobility.

It may be useful to consider the accuracy of the two solutions achieved, each with respect to their respective linearized Poisson's equation. For an exact solution the sum of the terms in the equation, denoted by $f(r)$, should equal zero. We have evaluated both differential equations with their corresponding solutions inserted. It was found, for large r, that $f(r)$ in our equation summed exactly to zero, while the CM terms evaluate to a small nonzero value. The explanation of these results is obvious. We used a $\kappa(r)[=\epsilon(r)]$ that is defined to be a constant for r greater than the screening radius of the dielectric function. Therefore, in this range $\kappa'(r)$ vanishes and the equation reduces exactly to the Dingle equation. This, of course, is the rationale behind our approximate boundary condition at r = 25 a.u., which we believe is physically reasonable though not, perhaps, mathematically rigorous. It might be remarked as a corollary that, in the case of other spatial dielectric functions that are not structured so as to limit exactly to a constant value, the validity of the approximation such as we used at r = 25 a.u. will be a function of the validity of the approximation that $\kappa'(r)$ is zero.

To continue with the examination of the CM case, we note that in the situation where an exact solution cannot be found, i.e., the sum of the terms in the equation is not equal to zero, the accuracy of the solution must be measured by the relation of $f(r)$ to the individual terms of the equation. Clearly, the relation of $|f(r)|$ to the largest term in $f(r)$ is the point of interest. We found that at r = 25 a.u. the value of f_{CM} was less than two orders of magnitude smaller than the largest term in their equation. This indicates an adequate but not an overwhelmingly accurate solution for large r. Our solution yielding an exact value for f_{SR} of zero, at large r, must be considered the more accurate representation in that region even though it is based on an approximate numerical boundary condition.

Finally, we would like to raise a question as to the relative numerical accuracies of the boundary conditions used by SR and by CM. Speaking with respect to a numerical solution, a boundary condition at infinity must be not only physically reasonable, it must be numerically expressible. That is, a boundary condition which asymptotes very slowly to some value at infinity is much less satisfactory for numerical solution schemes than is one which rapidly reaches to nearly its asymptotic value. We would contend that the approach of ϕ to ϕ_0 is much more rapid than is the approach of ϕ to zero. Thus, from such perspective, it is arguable that our boundary condition of $\phi = \phi_0$ at r = 25 a.u. is the more numerically feasible.

In summary, we assert that our boundary con-

dition at infinity, while lacking perhaps the theoretical rigor of CM's boundary condition, still contains a meaningful physical sense of the behavior of the impurity-ion potential. Additionally, our derived potential would seem to display the expected physical behavior which the CM potential lacks. However, as pointed out earlier by Meyer, any treatment of this problem must consider the solution of the nonlinearized Poisson's equation. Therefore, the most accurate information on the effect of the spatial variation of the dielectric function will not be produced by either impurity-ion potential.

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[10]G. Srinivasan, Phys. Rev. 178, 1244 (1969).