Potential Distribution and Capacitance of a Graded p-n Junction

By S. P. MORGAN and F. M. SMITS

(Manuscript received June 6, 1960)

For a graded p-n junction under sufficient forward bias, the usual space-charge approximation to the potential breaks down, and a numerical solution of the differential equation satisfied by the potential is required. A procedure is described which avoids the difficulties associated with direct numerical integration of the stiff differential equation, and which yields a pair of very close upper and lower bounds to the potential at all points. For a linearly graded junction, tables of bounds are given which nowhere differ by as much as 1 per cent, and which effectively bridge the gap between the space-charge case and the neutral case.

The computer solutions are used to calculate the voltage dependence of the stored charge (low-frequency ac capacitance) of a graded junction numerically, as a function of the bias voltage across the junction. The expression for the capacitance is split into two parts, one of which dominates in the neutral case and the other in the space-charge case. With properly normalized variables, it is possible to give a universal plot of small-signal ac capacitance against applied voltage. The results differ from the usual approximate formulas by amounts ranging up to nearly 10 per cent.

I. INTRODUCTION

In his theory of p-n junctions in semiconductors, Shockley[1] shows that the potential distribution in a linearly graded p-n junction satisfies a one-parameter differential equation of the form

$$\frac{d^2U}{dz^2} = \sinh U - Kz. \tag{1}$$

The solution of this nonlinear equation cannot be obtained by analytical methods. However, Shockley gives two approximations, each applicable in an extreme case. The space-charge approximation ($K \gg 1$) is valid in the case of a steep gradient at the junction, while the neutral approxi-

mation ($K \ll 1$) holds for a gentle gradient. Since in almost all cases of practical interest the gradients in p-n junctions are of such a magnitude that the space-charge approximation is valid, it has become the accepted form for the analysis of p-n junctions.

Shockley derived the differential equation (1) for the case of equilibrium — that is, for the case of zero bias across the junction. Recently Moll[2] has shown that the potential distribution in a p-n junction under bias satisfies the same one-parameter differential equation. The parameter K is now a function of the applied voltage, and it turns out that for most practical gradients in p-n junctions under forward bias the space-charge approximation ceases to be valid. For a proper description of the potential distribution in a biased junction, a numerical solution of (1) is required. Such a solution is obtained in the present paper and applied to the computation of the small-signal ac capacitance of the junction as a function of the bias voltage.

First Moll's derivation of the generalized differential equation for the potential distribution in a graded p-n junction under bias is reviewed. There follows a discussion of the physical principles which underlie the approximate solutions and the exact solution. Calculation of the exact solution by numerical integration, however, encounters the difficulty that one boundary condition is specified at infinity, and for large z the solutions found by ordinary numerical integration procedures diverge rapidly from the desired solution. This instability of the desired solution is called *stiffness*. An effective way to calculate the potential in spite of the stiffness consists in the computation of close upper and lower bounds, that is, two very nearby curves between which the actual potential must lie for all z. Mathematical details and extensive numerical tables are contained in Appendix A, while a graphical comparison between the exact space-charge distribution and the distribution assumed in the space-charge approximation is given in the body of the paper.

Finally the computer solutions are used to calculate the voltage dependence of the stored charge (low-frequency ac capacitance) of a graded junction. The results of the computation, which is described in Appendix B, yield a universal plot of the small-signal ac capacitance of the junction against applied voltage.

II. THE GENERALIZED DIFFERENTIAL EQUATION

To obtain the differential equation for the potential distribution in a biased junction, it is convenient to use the model of a p-n junction which was employed by Shockley in his derivation of the space-charge capacitance. The model (Fig. 1) assumes a linearly graded p-n junction in

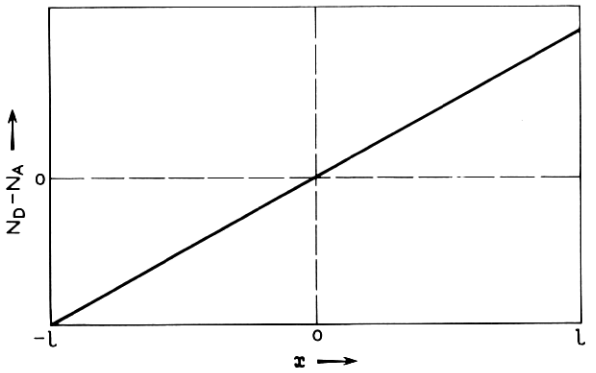

Fig. 1 — The pseudo-equilibrium model of a linearly graded junction.

which the net impurity concentration is given as $N_D - N_A = ax$, with N_D and N_A the density of donors and acceptors, respectively. Contacts are applied at $x = +l$ and $x = -l$. In the model the following processes are imagined to be prevented: (1) electron and hole recombination; (2) electron flow across the p-region contact at $x = -l$; (3) hole flow across the n-region contact at $x = +l$. Under such a pseudo-equilibrium condition, holes which flow in at $x = -l$ must remain in the structure; similarly, electrons flowing in at $x = +l$ must remain inside. No direct current is therefore possible, and the structure behaves like a capacitor.

If the potential of the p-region contact at $x = -l$ is increased by a voltage V with respect to the n-region contact, holes will flow into the specimen until the quasi-Fermi level φ_p for holes has increased by V, so that the holes inside are in equilibrium with the contact supplying the potential. A similar electron flow will occur at $x = +l$. In the pseudo-equilibrium state the quasi-Fermi levels for holes and electrons will have no gradient and will be separated by an amount equal to the applied voltage V.

In an actual p-n junction the region between $x = -l$ and $x = +l$ can be identified with the transition region. Under forward bias the current flow across the transition region gives rise to very small gradients in the quasi-Fermi levels, which can be neglected for a consideration of the potential distribution. Even for the derivation of the voltage-current characteristic, constant quasi-Fermi levels across the transition region are commonly assumed. The use of the pseudo-equilibrium model emphasizes the aspects of the transition region which are being considered here; this is particularly true in the derivation of the capacitance.

To derive the generalized differential equation, Boltzmann statistics

the problem is to find an integral curve of (A1) which passes through the origin with such a slope that at infinity it approaches the curve

$$\bar{U}(z) = \sinh^{-1} f(z); \tag{A3}$$

and in fact $U(z)$ must approach $\bar{U}(z)$ fast enough so that

$$\lim_{z\to\infty} [\sinh U(z) - \sinh \bar{U}(z)] = 0. \tag{A4}$$

One might, perhaps, be willing to take the existence of a physically meaningful solution of the boundary value problem for granted, on the ground that no matter how the fixed charge density $f(z)$ varies with position, the holes and electrons should be able to distribute themselves so that equilibrium is produced. A formal proof that the problem does indeed have a unique solution can be given under the assumptions that $f(z)$ is a nonnegative function with two continuous derivatives for $0 \leqq z < \infty$, that $\bar{U}(z)$ is everywhere concave downward, i.e.,

$$\bar{U}''(z) \leqq 0 \qquad \text{for} \quad 0 \leqq z < \infty, \tag{A5}$$

and that

$$\lim_{z\to\infty} \bar{U}''(z) = 0. \tag{A6}$$

Doubtless it would be sufficient to assume that $f(z)$ has only a finite number of finite discontinuities in $0 \leqq z < \infty$, and satisfies the given conditions for all sufficiently large z. We shall not take space to write out every detail of the proof, but the ideas are quite simple and will now be sketched as a basis for the following analysis and computations.

Typical integral curves of (A1) are shown in Fig. 7, these curves actually being computer solutions for the case $f(z) = 10z$. Let us denote by $U_s(z)$ the solution of (A1) which satisfies the initial conditions

$$U_s(0) = 0, \qquad U_s'(0) = s, \tag{A7}$$

where s is any real number. It is easily shown from the differential equation that if $s_2 > s_1$, then

$$U_{s_2}(z) - U_{s_1}(z) > (s_2 - s_1) \sinh z > 0, \tag{A8}$$

for any $z > 0$ for which $U_{s_2}(z)$ and $U_{s_1}(z)$ both exist.* We see from (A8) that $U_s(z)$ is an increasing function of s for fixed z, and that any two integral curves ultimately diverge with exponential speed.

* The solution $U_s(z)$ may become infinite as z approaches some finite value z_s, and so may not exist for $z \geqq z_s$. We shall not be concerned with such movable singularities, except to recognize that they can occur.

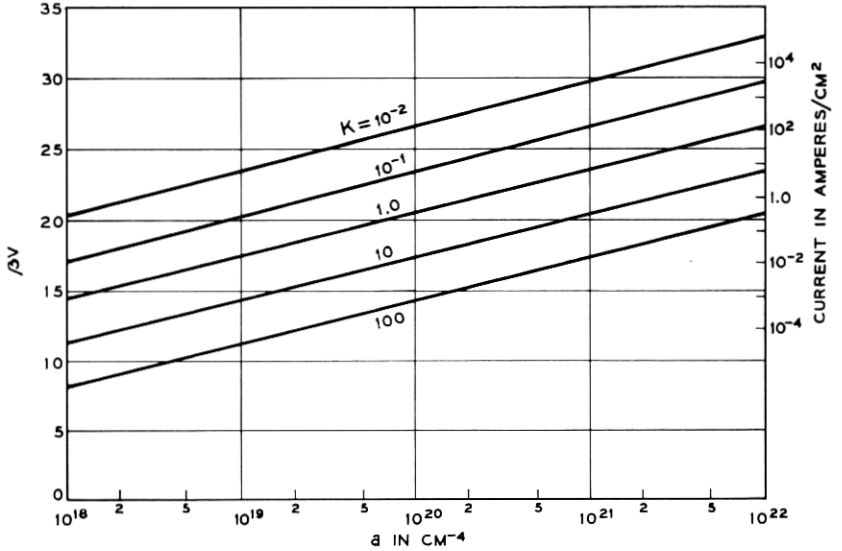

Fig. 2 — The parameter K as a function of forward bias and gradient at the junction.

one obtains for Poisson's equation the one-parameter differential equation

$$\frac{d^2U}{dz^2} = \sinh U - Kz. \tag{14}$$

For the case of zero bias, this differential equation corresponds to the one given by Shockley.* He gave two limiting approximations to the solution, namely the space-charge approximation for $K \gg 1$ and the neutral approximation for $K \ll 1$. Note, however, that on account of the factor $e^{-3\beta V/4}$ in the general expression for K as given by (13), K can pass through unity with increasing forward bias even if $K_0 \gg 1$.

To illustrate the effect of forward bias on K, Fig. 2, which is reproduced from Moll,[2] shows the values of K for practical gradients at the junction (values of a between 10^{18} and 10^{22} cm^{-4}) and for various values of forward bias. Also shown are reasonable estimates of current densities corresponding to such forward biases in practical cases. This plot dem-

* Shockley uses the normalized length coordinate $y = Kz$, so that (14) takes the form

$$\frac{d^2U}{dy^2} = \frac{1}{K^2}(\sinh U - y).$$

onstrates that one frequently encounters the condition where K is actually in the neighborhood of unity, in which case neither the space-charge approximation nor the neutral approximation is valid, and the exact solution is required.

Fig. 3 exhibits the relationships between the approximate solutions and the true solution. The figure is drawn for the intermediate case $K = 5$, and both the potential U and the charge density ρ are plotted against the normalized length coordinate z.

For the neutral approximation, one assumes $\rho \approx 0$ for all values of z.

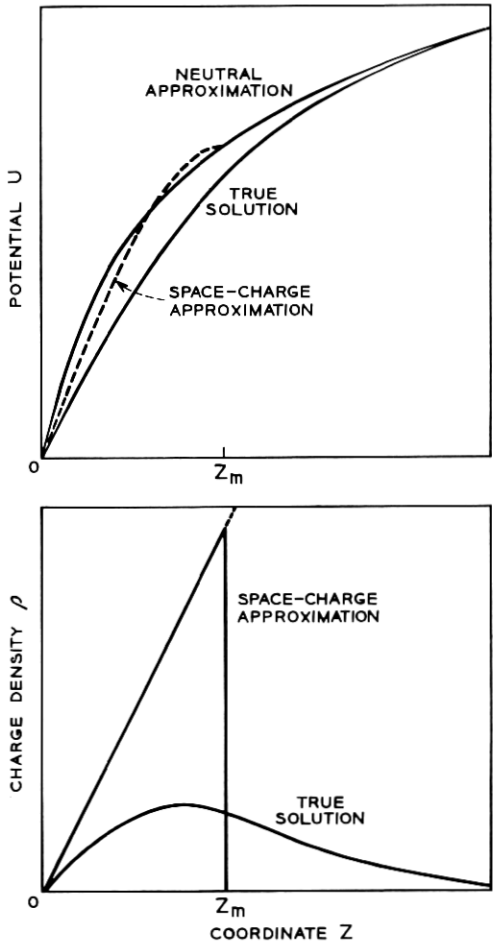

Fig. 3 — Relationships between the approximate solutions and the true solution for the case $K = 5$.

Then $d^2U/dz^2 \approx 0$, and the potential is approximately equal to the function

$$\bar{U} = \sinh^{-1}Kz. \tag{15}$$

For the space-charge approximation, one neglects the contribution of the mobile carriers to the charge density out to a point $|z| = z_m$, which is regarded as the edge of the space-charge region. Thus in the space-charge region one uses the differential equation

$$\frac{d^2U}{dz^2} = -Kz, \qquad |z| < z_m. \tag{16}$$

Beyond the point z_m one assumes neutrality and the potential is set equal to $\bar{U}$ as given by (15). At the point $z = z_m$, the two solutions join. One further condition is necessary to determine z_m; Shockley supplies this condition by requiring the space-charge solution to have zero slope at $z = z_m$. Since the neutral solution has a small positive slope at z_m, this method of joining results in a slight discontinuity in dU/dz at $z = z_m$. An improved method of joining would require that both the function and the first derivative be continuous at $z = z_m$. However, such a condition complicates the algebra without significantly improving the accuracy of the approximation.

The true solution is asymptotic to the neutral solution $\bar{U}$ as $z \to \infty$. The space-charge distribution will not have a sharp boundary, as is assumed in the space-charge approximation. A fraction of the fixed charges associated with the impurities are compensated by mobile carriers, giving rise to an actual net charge density like that indicated in the lower part of Fig. 3. Since for the exact solution the charge is distributed over a larger distance, the total charge must be smaller than is assumed in the space-charge approximation.

Calculation of the exact potential distribution in the junction involves numerical solution of the differential equation (14) subject to the boundary conditions $U = 0$ at $z = 0$ and $U \to \sinh^{-1}Kz$ as $z \to \infty$. The method of computation is described in Appendix A, where tables of upper and lower bounds for U which nowhere differ by as much as 1 per cent are given for 16 values of K ranging from 0.1 to 10,000.

The results of the calculations, for selected values of K, are also shown in terms of charge densities in Fig. 4. In this figure the fractional compensation of the fixed charges by mobile carriers, namely the ratio $(n - p)/(N_D - N_A)$, is plotted against z/z_m, where z_m is the space-charge width for the space-charge approximation. The value of z_m is plotted against K in Fig. 5. The normalization by z_m allows a complete representation of the results in one figure. It also readily permits a com-

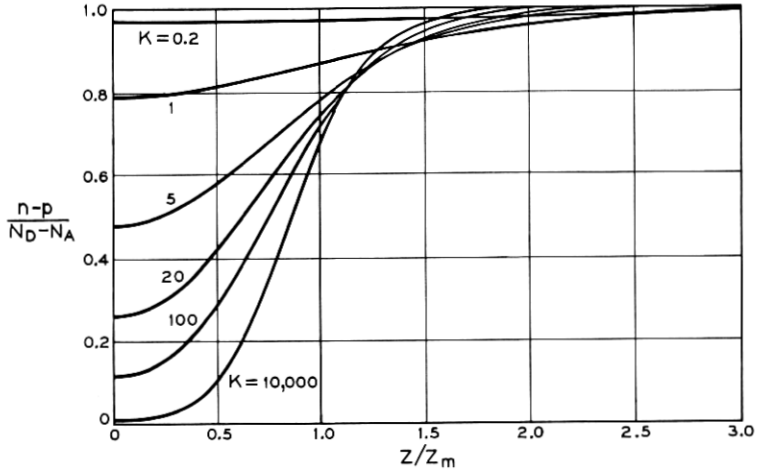

Fig. 4 — Fractional compensation of fixed charges by mobile carriers for various values of K.

parison between the true solution and the space-charge approximation, since for the latter the ordinate is zero for $z < z_m$ and unity for $z > z_m$.

It is apparent from Fig. 4 that the true solution differs markedly from the space-charge approximation, even for values of K as large as 10^4.

III. THE CAPACITANCE OF A GRADED p-n JUNCTION

The significant difference between the charge distribution assumed in the space-charge approximation and the actual charge distribution

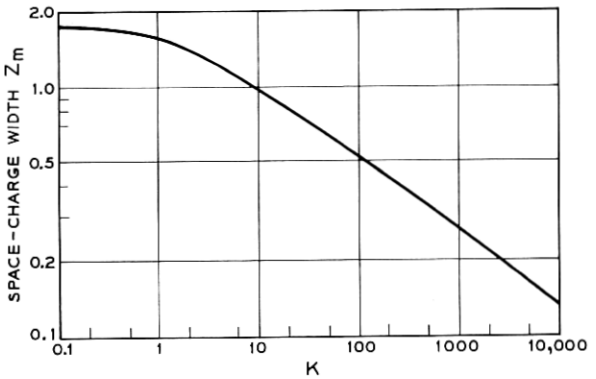

Fig. 5 — The space-charge width for the space-charge approximation.

prompted us to compute the voltage dependence of the stored charge (low-frequency ac capacitance) of a graded junction. For this problem the pseudo-equilibrium model is particularly helpful, since only capacitive currents will flow. A change in the voltage between the two contacts at $x = -l$ and $x = +l$ is associated with a change in the total number of mobile carriers stored in the structure. The total number of electrons and the total number of holes are always equal. The two types of carriers are equivalent to the charge on the two "plates" of the capacitor, and by considering the total number of holes one can express the capacitance as

$$C = \frac{d}{dV} q \left(\int_{-l}^{+l} p \, dx \right). \tag{17}$$

Because of the symmetry of the junction, the expression (17) can be written

$$C = \frac{d}{dV} \left(q \int_0^l (p + n) \, dx \right). \tag{18}$$

Since the density of fixed charges associated with the impurities is voltage-independent, one can rewrite this equation as

$$C = \frac{d}{dV} \left(q \int_0^l [(p + n) - (N_D - N_A)] \, dx \right). \tag{19}$$

After eliminating $N_D - N_A$ by (3), one obtains as the expression for the capacitance

$$C = \frac{d}{dV} \left(2q \int_0^l p \, dx \right) - \frac{d}{dV} \left(\int_0^l \rho \, dx \right). \tag{20}$$

The capacitance accordingly consists of two parts: the "neutral" capacitance

$$C_n = \frac{d}{dV} \left(2q \int_0^l p \, dx \right), \tag{21}$$

and the "space-charge" capacitance

$$C_\rho = -\frac{d}{dV} \left(\int_0^l \rho \, dx \right). \tag{22}$$

Since according to (13) the parameter K depends on V through the factor $e^{-3\beta V/4}$, one may express derivatives with respect to V in terms of derivatives with respect to K. Furthermore the expression for the space-charge capacitance converges very strongly as $l \to \infty$. Thus only a negligible error will be made if one replaces the upper limit of the in-

tegral by infinity. For the neutral capacitance, however, it is necessary to retain a finite value of l. After expressing p and ρ in terms of the potential by (2b) and (8) respectively, and transforming to dimensionless variables, one gets

$$C_n = \frac{C_0}{K^{\frac{1}{3}}}\left[\int_0^{z_l} e^{-U}dz + z_l e^{-U_l} - 3\,\frac{\partial}{\partial(\log K)}\int_0^{z_l} e^{-U}dz\right], \quad (23)$$

$$C_\rho = \frac{C_0}{K^{\frac{1}{3}}}\frac{\partial}{\partial z}\left[3\,\frac{\partial U}{\partial(\log K)} - U\right]_{z=0}. \quad (24)$$

In both cases C_0 is a normalizing capacitance given by

$$C_0 = \frac{\epsilon K_0^{\frac{1}{3}}}{4\mathfrak{L}_D}, \quad (25)$$

which involves only material constants and the gradient at the junction. For the space-charge capacitance, the expression multiplying C_0 is a function of K only. For the neutral capacitance, the multiplying function contains in addition the upper limit of the integral in (21), which can be expressed either by the actual coordinate l, by the normalized coordinate z_l, or by the normalized potential U_l of the electrode.

For $K \to 0$ the space-charge capacitance disappears and the relationship between U and K is given by (15). The neutral capacitance in this limit corresponds to the "capacitance for the neutral case" as described by Shockley,* and it takes the form

$$C_n \underset{K\to 0}{\approx} \frac{2U_l}{K^{\frac{1}{3}}}\,C_0. \quad (26)$$

For $K \gg 1$ the space-charge capacitance is much greater than the neutral capacitance. By using in (24) the functional relationship between U and K that results from the space-charge approximation, one obtains for the space-charge capacitance

$$C_\rho \approx \frac{2(3U_m)^{\frac{2}{3}}C_0}{3U_m \coth U_m - 1} \underset{K\to\infty}{\approx} \frac{2C_0}{(3U_m)^{\frac{1}{3}}}, \quad (27)$$

* In the present notation, Eq. (2.41) of Ref. 1 is equivalent to

$$C = \frac{(2U_l - 1)C_0}{K^{\frac{1}{3}}}.$$

A consistent retention of terms of order 1 in Shockley's derivation would, however, have led to a result exactly equivalent to (26) above. In particular it is necessary to write, for large x,

$$\exp(2\sinh^{-1} x) \approx 4x^2 + 2,$$

whereas Shockley effectively approximates this function by $4x^2$.

with U_m the normalized potential at the edge of the space-charge region, which is related to K by

$$K = \left(\frac{\sinh^3 U_m}{3U_m}\right)^{\frac{1}{2}}. \tag{28}$$

If one approximates $U_m = U_{m0} - \beta V/2$, where U_{m0} is the normalized potential at the edge of the space-charge region for zero bias, the last term of (27) agrees with the space-charge capacitance given by Shockley in Eq. (2.45) of Ref. 1.

The functions multiplying C_0 in (23) and (24) have been evaluated numerically, as described in Appendix B. In the expression for C_n a value of 10 has been used for U_l. (It should be emphasized that a fixed U_l does not correspond to a fixed l!) The results are shown in Fig. 6. Also shown are the approximations (26) and (27) for C_n and C_p respectively.

It may be noted that for large K the values for the exact space-charge capacitance fall above the approximate values. This at first appears surprising, since as mentioned above the total charge in the transition region is actually less than assumed under the space-charge approximation. However if one remembers that the validity of the approximation increases with increasing K, it becomes plausible that the change in total charge with K must be larger for the exact solution.

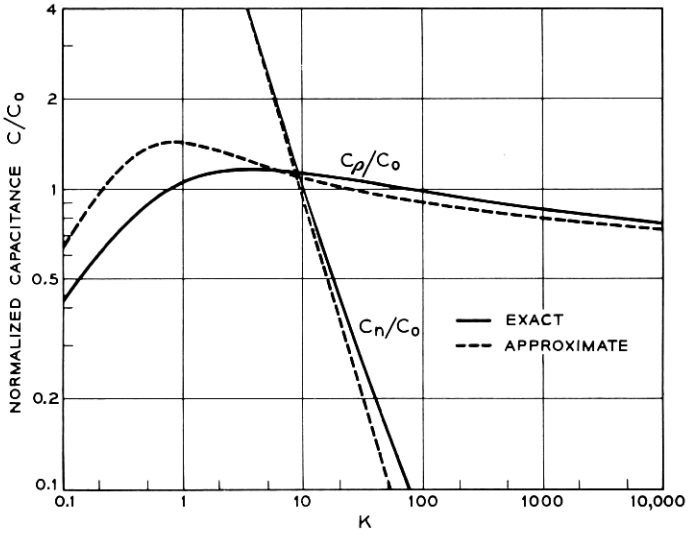

Fig. 6 — Approximate and exact values of the normalized neutral capacitance and the normalized space-charge capacitance.

The abscissa in Fig. 6 can be considered as a linear scale in $-V$, the applied voltage, with zero coinciding with the point $K = K_0$. Thus Fig. 6 may be used as a plot of the small-signal ac capacitance against voltage. In particular, it is apparent from Fig. 6 that in the range in which the neutral capacitance dominates, the approximation given by (26) is a good description of this capacitance. This finding is important, since in practical cases the value of U_l needs to be specified. One would choose as the boundary of the transition region a point up to which the assumption of constant quasi-Fermi levels is reasonably correct. Beyond this point one has to use the continuity equation to find the "diffusion" capacitance, which must be added to the capacitance of the transition region.

IV. ACKNOWLEDGMENTS

We wish to thank R. C. Prim for stimulating discussions of the mathematical aspects of this problem and for the use of his unpublished results. The numerical work has also had the benefit of unpublished investigations by A. Kooharian and W. L. Miranker.

APPENDIX A

Calculation of the Potential Distribution

We have to integrate numerically

$$U'' = \sinh U - f(z), \tag{A1}$$

where primes denote differentiation with respect to z, and $f(z)$ is a given function proportional to the density of fixed charge. For a linearly graded junction, of course, $f(z) = Kz$. In general, if $f(z)$ is an odd function of z, then $U(z)$ is an odd function of z, and we want a solution of (A1) satisfying the boundary conditions

$$U(0) = 0, \qquad \lim_{z\to\infty} U''(z) = 0. \tag{A2}$$

The second condition states that the total density of fixed plus mobile charges tends to zero at great distances from the junction.

A preliminary graphical treatment of (A1) is almost indispensable. Because of the first of the boundary conditions (A2), we need consider only the one-parameter family of integral curves passing through the origin with arbitrary slope. In view of the second boundary condition,

the problem is to find an integral curve of (A1) which passes through the origin with such a slope that at infinity it approaches the curve

$$\bar{U}(z) = \sinh^{-1} f(z); \tag{A3}$$

and in fact $U(z)$ must approach $\bar{U}(z)$ fast enough so that

$$\lim_{z\to\infty} [\sinh U(z) - \sinh \bar{U}(z)] = 0. \tag{A4}$$

One might, perhaps, be willing to take the existence of a physically meaningful solution of the boundary value problem for granted, on the ground that no matter how the fixed charge density $f(z)$ varies with position, the holes and electrons should be able to distribute themselves so that equilibrium is produced. A formal proof that the problem does indeed have a unique solution can be given under the assumptions that $f(z)$ is a nonnegative function with two continuous derivatives for $0 \leqq z < \infty$, that $\bar{U}(z)$ is everywhere concave downward, i.e.,

$$\bar{U}''(z) \leqq 0 \qquad \text{for} \quad 0 \leqq z < \infty, \tag{A5}$$

and that

$$\lim_{z\to\infty} \bar{U}''(z) = 0. \tag{A6}$$

Doubtless it would be sufficient to assume that $f(z)$ has only a finite number of finite discontinuities in $0 \leqq z < \infty$, and satisfies the given conditions for all sufficiently large z. We shall not take space to write out every detail of the proof, but the ideas are quite simple and will now be sketched as a basis for the following analysis and computations.

Typical integral curves of (A1) are shown in Fig. 7, these curves actually being computer solutions for the case $f(z) = 10z$. Let us denote by $U_s(z)$ the solution of (A1) which satisfies the initial conditions

$$U_s(0) = 0, \qquad U_s'(0) = s, \tag{A7}$$

where s is any real number. It is easily shown from the differential equation that if $s_2 > s_1$, then

$$U_{s_2}(z) - U_{s_1}(z) > (s_2 - s_1) \sinh z > 0, \tag{A8}$$

for any $z > 0$ for which $U_{s_2}(z)$ and $U_{s_1}(z)$ both exist.* We see from (A8) that $U_s(z)$ is an increasing function of s for fixed z, and that any two integral curves ultimately diverge with exponential speed.

* The solution $U_s(z)$ may become infinite as z approaches some finite value z_s, and so may not exist for $z \geqq z_s$. We shall not be concerned with such movable singularities, except to recognize that they can occur.

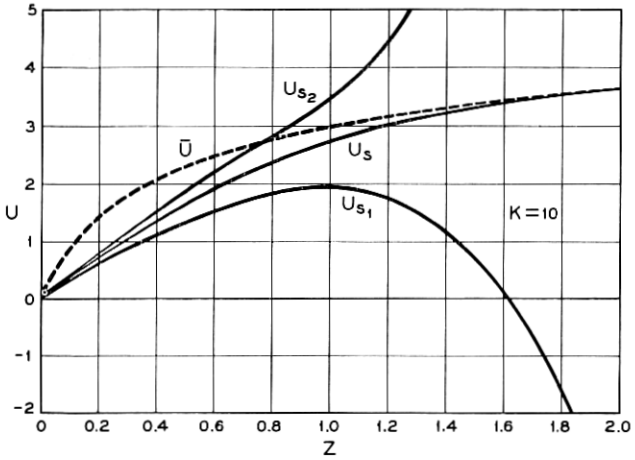

Fig. 7 — Integral curves of the differential equation $U'' = \sinh U - Kz$.

An integral curve which once crosses $\bar{U}(z)$ can never recross, since it has positive second derivative thenceforth, while by assumption $\bar{U}(z)$ has negative second derivative. Similarly, an integral curve which crosses the z-axis going downward has negative second derivative thenceforth, and can never recross the axis.

Now let us imagine, as is always possible, that we start with an initial slope s large enough so that $U_s(z)$ does cross $\bar{U}(z)$, and that we gradually decrease s until we come to the first integral curve that does not cross $\bar{U}(z)$ for any z. On the other hand we could start with a negative value of s, so that $U_s(z)$ surely lies below the z-axis, and increase s until we reach the first integral curve that does not lie below the z-axis anywhere. It turns out that these two distinguished integral curves are actually one and the same, so that the differential equation has exactly one solution which lies between $U = \bar{U}(z)$ and $U = 0$ for all z. (If there were two such solutions, by (A8) the distance between them would ultimately exceed $\bar{U}$.) We shall call this solution $U_S(z)$. It may be proved that $U_S(z)$ approaches $\bar{U}(z)$ and satisfies the boundary condition (A4) at infinity.

The object from now on is to find upper and lower bounds for the desired solution; that is, neighboring functions $U_+(z)$ and $U_-(z)$ such that

$$U_-(z) \leqq U_S(z) \leqq U_+(z) \qquad \text{for} \quad z \geqq 0. \tag{A9}$$

Clearly, if $s_1 < S < s_2$ then $U_{s_1}(z)$ is a lower bound and $U_{s_2}(z)$ is an upper bound; but according to (A8) these two curves are infinitely

far apart for infinite z. From the preceding discussion we know that $U_+(z) = \bar{U}(z)$ is always an upper bound and $U_-(z) = 0$ is always a lower bound. Furthermore, if $U_{1+}(z)$ and $U_{2+}(z)$ are upper bounds, then $\min [U_{1+}(z), U_{2+}(z)]$ is an upper bound; and if $U_{1-}(z)$ and $U_{2-}(z)$ are lower bounds, then $\max [U_{1-}(z), U_{2-}(z)]$ is a lower bound.

Given a lower bound $U_-(z)$, an upper bound may be constructed by two quadratures, as follows: Let

$$\begin{aligned} \eta''(z) &= \sinh U_-(z) - f(z), \\ \eta(0) &= 0, \\ \eta'(0) &= s, \end{aligned} \tag{A10}$$

and choose the initial slope s so that for some $z_m > 0$ we have

$$\eta(z_m) = \bar{U}(z_m). \tag{A11}$$

The upper bound is then

$$U_+(z) = \begin{cases} \eta(z), & 0 \leqq z \leqq z_m, \\ \bar{U}(z), & z > z_m. \end{cases} \tag{A12}$$

To prove that $\eta(z) \geqq U_S(z)$ for $0 \leqq z \leqq z_m$, we observe that the inequality is certainly satisfied at $z = 0$ and at $z = z_m$. If there were a subinterval in which $\eta(z) < U_S(z)$, then at some point z_1 of the subinterval we should have $\eta''(z_1) > U_S''(z_1)$, which is impossible in view of the differential equations (A1) and (A10). The contradiction establishes that $\eta(z)$ is an upper bound in $0 \leqq z \leqq z_m$.

Similarly, from a given upper bound $U_+(z)$ we can construct a lower bound by taking

$$\begin{aligned} \eta''(z) &= \sinh U_+(z) - f(z), \\ \eta(0) &= 0, \\ \eta'(0) &= s, \end{aligned} \tag{A13}$$

and choosing s so that for some $z_0 > 0$ we have

$$\eta'(z_0) = 0. \tag{A14}$$

The lower bound is then

$$U_-(z) = \begin{cases} \eta(z), & 0 \leqq z \leqq z_0, \\ \eta(z_0), & z > z_0; \end{cases} \tag{A15}$$

but it is not a very good bound because it is ultimately constant, while $U_S(z)$ may tend to infinity for large z.

The Shockley space-charge approximation may be obtained as an elementary upper bound, using (A10). Setting $U_-(z) = 0$, we get for a linearly graded junction with $f(z) = Kz$ an upper bound of the form

$$U_+(z) = \begin{cases} sz - Kz^3/6, & 0 \leqq z \leqq z_m, \\ \sinh^{-1} Kz, & z > z_m, \end{cases} \tag{A16}$$

where

$$sz_m - Kz_m^3/6 = \sinh^{-1} Kz_m . \tag{A17}$$

Since both s and z_m are disposable parameters, a second relationship may be imposed between them. Shockley requires the slope of the upper bound to vanish* at $z_m - 0$, so that

$$s - Kz_m^2/2 = 0. \tag{A18}$$

The solutions of (A17) and (A18) are then expressed, in terms of a parameter U_m which satisfies

$$\left(\frac{\sinh^3 U_m}{3U_m}\right)^{\frac{1}{2}} = K, \tag{A19}$$

by the equations

$$\begin{aligned} z_m &= \frac{\sinh U_m}{K}, \\ s &= \frac{\sinh^2 U_m}{2K}. \end{aligned} \tag{A20}$$

The space-charge width z_m, which was plotted in Fig. 5, is tabulated in Table I as a function of K, together with the initial slope s according to the space-charge approximation, and the initial slope S obtained by the numerical method described below.

Unfortunately it does not appear to be possible to converge on the desired solution $U_S(z)$ by repeated applications of (A10) and (A13). A limited amount of numerical experimentation suggests that iteration, even starting from a bound which is known to be very close to $U_S(z)$, rapidly leads to a particular pair of curves which are a finite distance apart for every $z > 0$. Although it is possible, as Prim[3] and Morrison[4] have shown, to obtain a number of analytic upper and lower bounds for $U_S(z)$ of varying degrees of complexity, the most practical way of actually computing close upper and lower bounds seems to be in terms of integral curves of the differential equation itself. Thus let $U_{s_2}(z)$ be an

* A slightly better bound would be obtained by making the slope of $U_+(z)$ continuous at z_m.

TABLE I—SPACE-CHARGE WIDTH AND INITIAL SLOPE OF $U(z)$

K	Space-Charge Approximation		Exact Solution
	z_m	s	S
0.1	1.7278	0.14926	0.099094
0.2	1.7158	0.29440	0.19402
0.5	1.6535	0.68348	0.44698
1	1.5396	1.1852	0.78927
2	1.3760	1.8935	1.3134
5	1.1350	3.2206	2.3792
10	0.9610	4.6180	3.5599
20	0.8046	6.4737	5.1709
50	0.6287	9.8810	8.1895
100	0.5183	13.432	11.379
200	0.4255	18.108	15.614
500	0.3262	26.610	23.378
1000	0.2660	35.389	31.449
2000	0.2165	46.864	42.049
5000	0.1644	67.568	61.264
10000	0.1333	88.791	81.052

integral curve of (A1) which passes through the origin with some initial slope s_2 and crosses $\bar{U}(z)$ at some point z_0. Then an upper bound for $U_S(z)$ is given by

$$U_+(z) = \begin{cases} U_{s_2}(z), & 0 \leqq z \leqq z_0, \\ \bar{U}(z), & z > z_0. \end{cases} \tag{A21}$$

Similarly a lower bound may be constructed from any integral curve $U_{s_1}(z)$ which starts with a positive slope s_1 but ultimately turns downward. Ordinarily we do not have to follow $U_{s_1}(z)$ beyond the point where its slope is zero. Let us introduce the auxiliary function

$$U_{-1}(z) = \sinh^{-1}[f(z) + \bar{U}''(z)]. \tag{A22}$$

$U_{-1}(z)$ is a known function of z which approaches $\bar{U}(z)$ from below for large z as $\bar{U}''(z)$ approaches zero; it is plotted in Fig. 8 for the case $f(z) = 10z$. Now suppose that for some positive z_0 we have

$$\bar{U}(z) - U_{-1}(z) \leqq \epsilon_0 \quad \text{for} \quad z \geqq z_0, \tag{A23}$$

where

$$\epsilon_0 = \bar{U}(z_0) - U_{s_1}(z_0). \tag{A24}$$

Then a lower bound for $U_S(z)$ is given by

$$U_-(z) = \begin{cases} U_{s_1}(z), & 0 \leqq z \leqq z_0, \\ \bar{U}(z) - \epsilon_0, & z > z_0. \end{cases} \tag{A25}$$

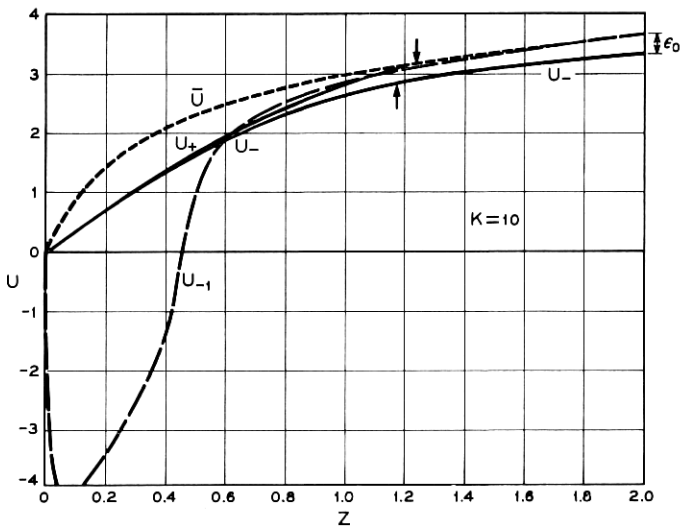

Fig. 8 — Upper and lower bounds, together with the curves $\bar{U}(z)$ and $U_{-1}(z)$.

In other words, $U_S(z)$ lies in a strip of constant width ϵ_0 below $\bar{U}(z)$ for $z \geqq z_0$.

To prove the last statement, define

$$\epsilon(z) = \bar{U}(z) - U_S(z). \tag{A26}$$

Since $U_{s_1}(z)$ ultimately turns downward, we know that it lies below $U_S(z)$ at $z = z_0$. We also know that $U_S(z)$ approaches $\bar{U}(z)$ at infinity, so

$$\epsilon(z_0) < \epsilon_0 \qquad \text{and} \qquad \lim_{z\to\infty} \epsilon(z) = 0. \tag{A27}$$

It follows that if there were some interval beyond z_0 in which $\epsilon(z) > \epsilon_0$, there would be some point z_1 of the interval at which $\epsilon''(z_1) < 0$. But at this point we have

$$\begin{aligned} \epsilon''(z_1) &= \bar{U}''(z_1) - U_S''(z_1) \\ &= \sinh U_{-1}(z_1) - \sinh U_S(z_1) > 0, \end{aligned} \tag{A28}$$

since, by (A23), $U_S(z_1) < U_{-1}(z_1)$ if $\bar{U}(z_1) - U_S(z_1) > \epsilon_0$. This contradiction proves the theorem.

In practice it is usually possible to choose z_0 to minimize the distance between $U_{s_1}(z)$ and $\bar{U}(z)$, i.e., so that

$$U'_{s_1}(z_0) = \bar{U}'(z_0). \tag{A29}$$

However, this condition is not required for the preceding proof.

Representative upper and lower bounds obtained in this way for $K = 10$ are shown in Fig. 8, together with the curves $\bar{U}(z)$ and $U_{-1}(z)$. For ease in plotting, the value of ϵ_0 has been chosen larger than would be necessary to accept in a practical case. The vertical arrows indicate, respectively, the point at which U_+ becomes $\bar{U}$ and the point at which U_- becomes $\bar{U} - \epsilon_0$.

To mechanize the computation of upper and lower bounds, one has only to integrate (A1) numerically, starting from the origin with a given slope, out to the point where the integral curve identifies itself either by crossing $\bar{U}(z)$ or by attaining zero slope. The initial slope is then adjusted (downward in the former case, upward in the latter), and the process repeated until the bounds nowhere differ by more than a preassigned amount. This approach may be called the "sweep method."

Any standard procedure may be used for the numerical integration. We took the fourth-order Runge-Kutta method,[5] adapted for an equation of the form $y'' = f(x, y)$. In practice the IBM 704 was supplied with the value of K, an initial guess at the slope s, and criteria for stopping; integral curves could be run off at the rate of several per minute.

The criterion for refinement of a particular solution was more or less arbitrarily taken to be the determination of the initial slope to five significant figures.* This led to upper and lower bounds which differ by less than 1 per cent of their mean value in all cases. Typical plots are shown in Figs. 9, 10, and 11. In Fig. 9, where K has the small value 0.1, the solution $U_S(z)$ nowhere differs from $\bar{U}(z)$ by more than 1 per cent, and no attempt has been made to plot the two curves separately. Fig. 10 represents the intermediate value $K = 10$, and Fig. 11 the large value $K = 10{,}000$. The difference between upper and lower bounds for a given K, while obvious in the tabulated values near the upper end of the range of z, is too small to be conveniently plotted on these figures.

Table II shows $\bar{U}(z)$, $U_+(z)$, and $U_-(z)$ for 16 values of K ranging from 0.1 to 10,000. The values of $U_+(z)$ and $U_-(z)$, considered as numerical solutions of the differential equation (A1), are believed to be accurate, with a few possible exceptions, to the four decimal places shown.

* More precisely, $U_+'(0)$ exceeds $U_-'(0)$ by one unit of the fifth significant figure, where $U_+'(0)$ is given as S in Table I.

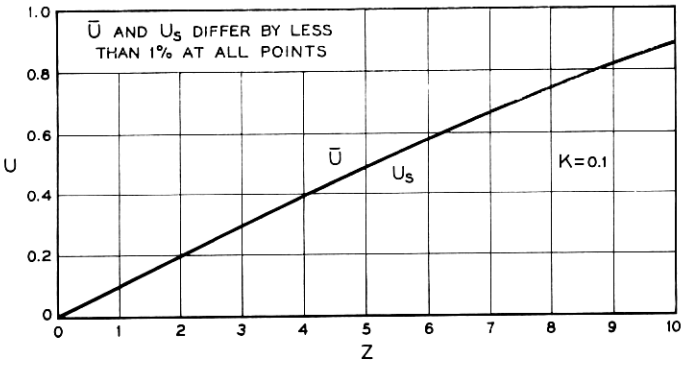

Fig. 9 — Potential distribution $U(z)$ for $K = 0.1$.

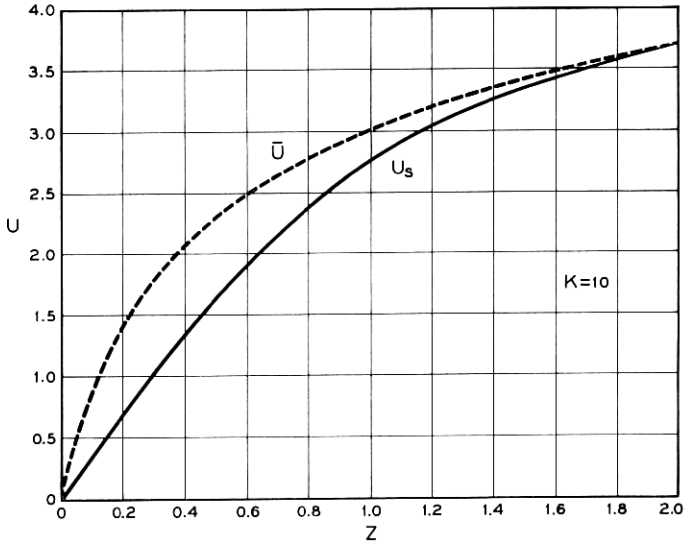

Fig. 10 — Potential distribution $U(z)$ for $K = 10$.

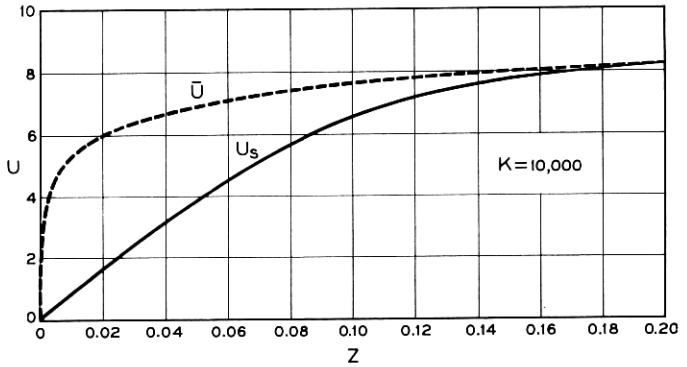

Fig. 11 — Potential distribution $U(z)$ for $K = 10{,}000$.

TABLE II — THE FUNCTIONS $\bar{U}(z)$, $U_+(z)$, AND $U_-(z)$

$K = 0.1$

z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.
0.500	0.0500	0.0495	0.0495
1.000	0.0998	0.0989	0.0989
1.500	0.1494	0.1481	0.1481
2.000	0.1987	0.1970	0.1970
2.500	0.2475	0.2454	0.2454
3.000	0.2957	0.2933	0.2933
3.500	0.3432	0.3406	0.3406
4.000	0.3900	0.3872	0.3872
4.500	0.4360	0.4331	0.4331
5.000	0.4812	0.4782	0.4782
5.500	0.5255	0.5224	0.5224
6.000	0.5688	0.5657	0.5657
6.500	0.6112	0.6081	0.6081
7.000	0.6527	0.6496	0.6496
7.500	0.6931	0.6902	0.6901
8.000	0.7327	0.7299	0.7297
8.500	0.7712	0.7686	0.7683
9.000	0.8089	0.8066	0.8059**
9.500	0.8456	0.8437	0.8426**
10.000	0.8814	0.8803	0.8784**
10.500	0.9163	0.9163*	0.9134**

* $\bar{U}(z)$ ** $\bar{U}(z) - 0.0029$

$K = 0.2$

z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.
0.200	0.0400	0.0388	0.0388
0.400	0.0799	0.0775	0.0775
0.600	0.1197	0.1162	0.1162
0.800	0.1593	0.1547	0.1547
1.000	0.1987	0.1930	0.1930
1.200	0.2378	0.2311	0.2311
1.400	0.2765	0.2690	0.2689
1.600	0.3148	0.3065	0.3064
1.800	0.3526	0.3436	0.3436
2.000	0.3900	0.3804	0.3804
2.200	0.4269	0.4168	0.4167
2.400	0.4633	0.4527	0.4526
2.600	0.4990	0.4881	0.4881
2.800	0.5342	0.5231	0.5230
3.000	0.5688	0.5576	0.5575
3.200	0.6028	0.5915	0.5914
3.400	0.6362	0.6249	0.6248
3.600	0.6690	0.6578	0.6576
3.800	0.7011	0.6901	0.6898
4.000	0.7327	0.7218	0.7215
4.200	0.7636	0.7530	0.7526
4.400	0.7939	0.7837	0.7832
4.600	0.8237	0.8138	0.8132
4.800	0.8528	0.8434	0.8426
5.000	0.8814	0.8724	0.8715
5.200	0.9094	0.9010	0.8998
5.400	0.9368	0.9290	0.9275
5.600	0.9637	0.9567	0.9547
5.800	0.9901	0.9838	0.9814
6.000	1.0160	1.0106	1.0075
6.200	1.0413	1.0371	1.0331
6.400	1.0662	1.0633	1.0581
6.600	1.0906	1.0894	1.0827
6.800	1.1145	1.1145*	1.1067
7.000	1.1380	1.1380*	1.1302**

* $\bar{U}(z)$ ** $\bar{U}(z) - 0.0078$

$K = 0.5$

z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.
0.200	0.0998	0.0893	0.0893
0.400	0.1987	0.1782	0.1782
0.600	0.2957	0.2663	0.2663
0.800	0.3900	0.3532	0.3531
1.000	0.4812	0.4384	0.4384
1.200	0.5688	0.5218	0.5218
1.400	0.6527	0.6030	0.6030
1.600	0.7327	0.6819	0.6819
1.800	0.8089	0.7582	0.7581

$K = 1.0$

z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.
0.200	0.1987	0.1576	0.1576
0.400	0.3900	0.3135	0.3135
0.600	0.5688	0.4662	0.4661
0.800	0.7327	0.6142	0.6142
1.000	0.8814	0.7564	0.7563
1.200	1.0160	0.8918	0.8918
1.400	1.1380	1.0198	1.0198
1.600	1.2490	1.1401	1.1401
1.800	1.3504	1.2526	1.2526

TABLE II — *Continued*

$K = 0.5$				$K = 1.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$	z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
2.000	0.8814	0.8318	0.8317	2.000	1.4436	1.3574	1.3573
2.200	0.9503	0.9026	0.9026	2.200	1.5297	1.4547	1.4546
2.400	1.0160	0.9707	0.9706	2.400	1.6094	1.5450	1.5450
2.600	1.0785	1.0360	1.0359	2.600	1.6837	1.6289	1.6288
2.800	1.1380	1.0985	1.0984	2.800	1.7532	1.7068	1.7066
3.000	1.1948	1.1584	1.1583	3.000	1.8184	1.7792	1.7790
3.200	1.2490	1.2157	1.2155	3.200	1.8799	1.8468	1.8465
3.400	1.3008	1.2705	1.2703	3.400	1.9379	1.9101	1.9097
3.600	1.3504	1.3230	1.3227	3.600	1.9928	1.9694	1.9688
3.800	1.3980	1.3732	1.3728	3.800	2.0450	2.0253	2.0245
4.000	1.4436	1.4213	1.4208	4.000	2.0947	2.0780	2.0769
4.200	1.4875	1.4675	1.4668	4.200	2.1421	2.1281	2.1263
4.400	1.5297	1.5118	1.5109	4.400	2.1874	2.1757	2.1731
4.600	1.5703	1.5543	1.5532	4.600	2.2308	2.2213	2.2173
4.800	1.6094	1.5953	1.5937	4.800	2.2724	2.2651	2.2591**
5.000	1.6472	1.6349	1.6327	5.000	2.3124	2.3074	2.2991**
5.200	1.6837	1.6731	1.6700	5.200	2.3509	2.3487	2.3376**
5.400	1.7191	1.7101	1.7059	5.400	2.3880	2.3880*	2.3747**
5.600	1.7532	1.7461	1.7403**				
5.800	1.7863	1.7813	1.7734**				
6.000	1.8184	1.8158	1.8055**				
6.200	1.8496	1.8496*	1.8366**				
* $\bar{U}(z)$		** $\bar{U}(z) - 0.0130$		* $\bar{U}(z)$		** $\bar{U}(z) - 0.0134$	

$K = 2.0$				$K = 5.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$	z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.	0.	0.	0.	0.
0.100	0.1987	0.1312	0.1312	0.100	0.4812	0.2375	0.2375
0.200	0.3900	0.2618	0.2617	0.200	0.8814	0.4724	0.4724
0.300	0.5688	0.3910	0.3909	0.300	1.1948	0.7022	0.7022
0.400	0.7327	0.5182	0.5181	0.400	1.4436	0.9246	0.9246
0.500	0.8814	0.6428	0.6427	0.500	1.6472	1.1377	1.1377
0.600	1.0160	0.7643	0.7642	0.600	1.8184	1.3399	1.3398
0.700	1.1380	0.8822	0.8822	0.700	1.9657	1.5298	1.5297
0.800	1.2490	0.9962	0.9961	0.800	2.0947	1.7068	1.7067
0.900	1.3504	1.1058	1.1057	0.900	2.2093	1.8705	1.8704
1.000	1.4436	1.2109	1.2108	1.000	2.3124	2.0208	2.0207
1.100	1.5297	1.3114	1.3112	1.100	2.4061	2.1583	2.1582
1.200	1.6094	1.4070	1.4068	1.200	2.4918	2.2835	2.2833
1.300	1.6837	1.4978	1.4976	1.300	2.5708	2.3972	2.3970
1.400	1.7532	1.5839	1.5836	1.400	2.6441	2.5005	2.5002
1.500	1.8184	1.6653	1.6650	1.500	2.7125	2.5943	2.5939
1.600	1.8799	1.7422	1.7419	1.600	2.7765	2.6796	2.6792
1.700	1.9379	1.8148	1.8144	1.700	2.8367	2.7576	2.7569
1.800	1.9928	1.8832	1.8828	1.800	2.8934	2.8289	2.8281
1.900	2.0450	1.9478	1.9473	1.900	2.9472	2.8947	2.8936
2.000	2.0947	2.0088	2.0082	2.000	2.9982	2.9555	2.9541
2.100	2.1421	2.0663	2.0656	2.100	3.0468	3.0121	3.0102
2.200	2.1874	2.1207	2.1198	2.200	3.0931	3.0651	3.0625
2.300	2.2308	2.1721	2.1711	2.300	3.1374	3.1151	3.1115

TABLE II — *Continued*

$K = 2.0$				$K = 5.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$	z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
2.400	2.2724	2.2209	2.2197	2.400	3.1798	3.1625	3.1576
2.500	2.3124	2.2672	2.2657	2.500	3.2205	3.2078	3.2010
2.600	2.3509	2.3113	2.3094	2.600	3.2596	3.2516	3.2420
2.700	2.3880	2.3533	2.3509	2.700	3.2972	3.2943	3.2807
2.800	2.4238	2.3934	2.3905	2.800	3.3335	3.3335*	3.3172**
2.900	2.4584	2.4318	2.4282				
3.000	2.4918	2.4687	2.4641				
3.100	2.5241	2.5042	2.4984				
3.200	2.5555	2.5384	2.5310				
3.300	2.5859	2.5716	2.5621				
3.400	2.6154	2.6038	2.5917**				
3.500	2.6441	2.6352	2.6204**				
3.600	2.6720	2.6660	2.6483**				
3.700	2.6992	2.6964	2.6755**				
3.800	2.7256	2.7256*	2.7019**				
* $\bar{U}(z)$		** $\bar{U}(z) - 0.0237$		* $\bar{U}(z)$		** $\bar{U}(z) - 0.0163$	

$K = 10.0$				$K = 20.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$	z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.	0.	0.	0.	0.
0.100	0.8814	0.3549	0.3549	0.100	1.4436	0.5146	0.5146
0.200	1.4436	0.7035	0.7035	0.200	2.0947	1.0147	1.0147
0.300	1.8184	1.0398	1.0397	0.300	2.4918	1.4870	1.4870
0.400	2.0947	1.3585	1.3585	0.400	2.7765	1.9206	1.9205
0.500	2.3124	1.6555	1.6554	0.500	2.9982	2.3079	2.3078
0.600	2.4918	1.9278	1.9278	0.600	3.1798	2.6453	2.6452
0.700	2.6441	2.1739	2.1739	0.700	3.3335	2.9330	2.9329
0.800	2.7765	2.3935	2.3934	0.800	3.4667	3.1746	3.1745
0.900	2.8934	2.5875	2.5874	0.900	3.5843	3.3756	3.3755
1.000	2.9982	2.7576	2.7575	1.000	3.6895	3.5427	3.5424
1.100	3.0931	2.9063	2.9060	1.100	3.7847	3.6823	3.6820
1.200	3.1798	3.0361	3.0358	1.200	3.8716	3.8005	3.8000
1.300	3.2596	3.1497	3.1494	1.300	3.9516	3.9020	3.9012
1.400	3.3335	3.2498	3.2493	1.400	4.0257	3.9910	3.9896
1.500	3.4023	3.3386	3.3379	1.500	4.0946	4.0702	4.0680
1.600	3.4667	3.4181	3.4171	1.600	4.1591	4.1423	4.1385
1.700	3.5272	3.4900	3.4885	1.700	4.2197	4.2089	4.2024
1.800	3.5843	3.5556	3.5534	1.800	4.2769	4.2719	4.2604**
1.900	3.6383	3.6161	3.6128	1.900	4.3309	4.3309*	4.3145**
2.000	3.6895	3.6723	3.6673				
2.100	3.7382	3.7252	3.7175				
2.200	3.7847	3.7754	3.7640**				
2.300	3.8291	3.8235	3.8084**				
2.400	3.8716	3.8704	3.8509**				
2.500	3.9124	3.9124*	3.8917**				
* $\bar{U}(z)$		** $\bar{U}(z) - 0.0207$		* $\bar{U}(z)$		** $\bar{U}(z) - 0.0164$	

TABLE II — *Continued*

$K = 50.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.
0.050	1.6472	0.4086	0.4086
0.100	2.3124	0.8120	0.8120
0.150	2.7125	1.2052	1.2052
0.200	2.9982	1.5835	1.5835
0.250	3.2205	1.9427	1.9427
0.300	3.4023	2.2793	2.2792
0.350	3.5562	2.5905	2.5904
0.400	3.6895	2.8746	2.8745
0.450	3.8072	3.1309	3.1308
0.500	3.9124	3.3595	3.3595
0.550	4.0077	3.5617	3.5616
0.600	4.0946	3.7391	3.7390
0.650	4.1746	3.8941	3.8940
0.700	4.2487	4.0293	4.0291
0.750	4.3177	4.1471	4.1470
0.800	4.3822	4.2503	4.2501
0.850	4.4428	4.3411	4.3408
0.900	4.4999	4.4215	4.4211
0.950	4.5540	4.4935	4.4930
1.000	4.6053	4.5584	4.5577
1.050	4.6541	4.6176	4.6167
1.100	4.7006	4.6721	4.6708
1.150	4.7450	4.7228	4.7209
1.200	4.7876	4.7703	4.7675
1.250	4.8284	4.8152	4.8111
1.300	4.8676	4.8580	4.8520
1.350	4.9053	4.8993	4.8904
1.400	4.9417	4.9396	4.9268**
1.450	4.9768	4.9768*	4.9619**

* $\bar{U}(z)$ ** $\bar{U}(z) - 0.0149$

$K = 100.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.
0.050	2.3124	0.5671	0.5671
0.100	2.9982	1.1232	1.1231
0.150	3.4023	1.6579	1.6578
0.200	3.6895	2.1615	2.1613
0.250	3.9124	2.6260	2.6257
0.300	4.0946	3.0454	3.0451
0.350	4.2487	3.4162	3.4158
0.400	4.3822	3.7378	3.7373
0.450	4.4999	4.0120	4.0114
0.500	4.6053	4.2429	4.2422
0.550	4.7006	4.4358	4.4349
0.600	4.7876	4.5968	4.5956
0.650	4.8676	4.7316	4.7299
0.700	4.9417	4.8458	4.8433
0.750	5.0107	4.9438	4.9403
0.800	5.0752	5.0297	5.0244
0.850	5.1358	5.1066	5.0986
0.900	5.1930	5.1774	5.1649
0.950	5.2471	5.2471*	5.2250
1.000	5.2983	5.2983*	5.2799
1.050	5.3471	5.3471*	5.3301
1.100	5.3936	5.3936*	5.3767**

* $\bar{U}(z)$ ** $\bar{U}(z) - 0.0170$

$K = 200.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.
0.020	2.0947	0.3120	0.3120
0.040	2.7765	0.6226	0.6226
0.060	3.1798	0.9302	0.9302
0.080	3.4667	1.2335	1.2334
0.100	3.6895	1.5310	1.5309
0.120	3.8716	1.8214	1.8212
0.140	4.0257	2.1034	2.1032
0.160	4.1591	2.3758	2.3756
0.180	4.2769	2.6375	2.6373
0.200	4.3822	2.8877	2.8875
0.220	4.4775	3.1254	3.1252
0.240	4.5645	3.3501	3.3499
0.260	4.6445	3.5613	3.5611
0.280	4.7186	3.7588	3.7585

$K = 500.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.
0.020	2.9982	0.4669	0.4669
0.040	3.6895	0.9300	0.9300
0.060	4.0946	1.3856	1.3855
0.080	4.3822	1.8299	1.8298
0.100	4.6053	2.2595	2.2594
0.120	4.7876	2.6709	2.6708
0.140	4.9417	3.0613	3.0612
0.160	5.0752	3.4280	3.4278
0.180	5.1930	3.7689	3.7687
0.200	5.2983	4.0825	4.0823
0.220	5.3936	4.3680	4.3678
0.240	5.4807	4.6254	4.6251
0.260	5.5607	4.8552	4.8549
0.280	5.6348	5.0588	5.0584

TABLE II — *Continued*

$K = 200.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.300	4.7876	3.9425	3.9421
0.320	4.8521	4.1125	4.1121
0.340	4.9127	4.2691	4.2687
0.360	4.9699	4.4128	4.4123
0.380	5.0239	4.5442	4.5437
0.400	5.0752	4.6640	4.6635
0.420	5.1240	4.7731	4.7725
0.440	5.1705	4.8722	4.8715
0.460	5.2150	4.9622	4.9614
0.480	5.2575	5.0440	5.0431
0.500	5.2983	5.1185	5.1174
0.520	5.3376	5.1863	5.1850
0.540	5.3753	5.2483	5.2467
0.560	5.4117	5.3051	5.3033
0.580	5.4468	5.3574	5.3552
0.600	5.4807	5.4057	5.4030
0.620	5.5134	5.4506	5.4473
0.640	5.5452	5.4924	5.4884
0.660	5.5760	5.5316	5.5267
0.680	5.6058	5.5685	5.5624
0.700	5.6348	5.6034	5.5958
0.720	5.6630	5.6365	5.6270
0.740	5.6904	5.6682	5.6562
0.760	5.7170	5.6986	5.6834**
0.780	5.7430	5.7278	5.7094**
0.800	5.7683	5.7561	5.7347**
0.820	5.7930	5.7836	5.7594**
0.840	5.8171	5.8105	5.7835**
0.860	5.8406	5.8370	5.8070**
0.880	5.8636	5.8636*	5.8300**

* $\bar{U}(z)$ ** $\bar{U}(z) - 0.0336$

$K = 500.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.300	5.7038	5.2378	5.2374
0.320	5.7683	5.3946	5.3941
0.340	5.8290	5.5313	5.5308
0.360	5.8861	5.6506	5.6499
0.380	5.9402	5.7547	5.7539
0.400	5.9915	5.8460	5.8450
0.420	6.0403	5.9264	5.9251
0.440	6.0868	5.9978	5.9961
0.460	6.1312	6.0616	6.0594
0.480	6.1738	6.1192	6.1163
0.500	6.2146	6.1718	6.1678
0.520	6.2538	6.2201	6.2147
0.540	6.2916	6.2649	6.2577
0.560	6.3279	6.3069	6.2970
0.580	6.3630	6.3466	6.3329**
0.600	6.3969	6.3843	6.3668**
0.620	6.4297	6.4206	6.3996**
0.640	6.4615	6.4557	6.4313**
0.660	6.4922	6.4902	6.4621**
0.680	6.5221	6.5221*	6.4920**

* $\bar{U}(z)$ ** $\bar{U}(z) - 0.0301$

$K = 1000.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.
0.020	3.6895	0.6277	0.6277
0.040	4.3822	1.2477	1.2476
0.060	4.7876	1.8523	1.8522
0.080	5.0752	2.4342	2.4341
0.100	5.2983	2.9864	2.9863
0.120	5.4807	3.5027	3.5025
0.140	5.6348	3.9777	3.9775
0.160	5.7683	4.4075	4.4073
0.180	5.8861	4.7899	4.7897
0.200	5.9915	5.1245	5.1243
0.220	6.0868	5.4128	5.4126
0.240	6.1738	5.6582	5.6579
0.260	6.2538	5.8649	5.8645
0.280	6.3279	6.0381	6.0376
0.300	6.3969	6.1831	6.1825
0.320	6.4615	6.3049	6.3041

$K = 2000.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.
0.010	3.6895	0.4202	0.4202
0.020	4.3822	0.8384	0.8384
0.030	4.7876	1.2527	1.2526
0.040	5.0752	1.6611	1.6611
0.050	5.2983	2.0619	2.0618
0.060	5.4807	2.4530	2.4529
0.070	5.6348	2.8327	2.8326
0.080	5.7683	3.1992	3.1991
0.090	5.8861	3.5510	3.5509
0.100	5.9915	3.8866	3.8865
0.110	6.0868	4.2046	4.2044
0.120	6.1738	4.5039	4.5038
0.130	6.2538	4.7838	4.7837
0.140	6.3279	5.0438	5.0436
0.150	6.3969	5.2834	5.2833
0.160	6.4615	5.5030	5.5028

TABLE II — *Continued*

$K = 1000.0$				$K = 2000.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$	z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.340	6.5221	6.4082	6.4071	0.170	6.5221	5.7029	5.7027
0.360	6.5793	6.4967	6.4952	0.180	6.5793	5.8838	5.8836
0.380	6.6333	6.5738	6.5716	0.190	6.6333	6.0466	6.0464
0.400	6.6846	6.6420	6.6390	0.200	6.6846	6.1926	6.1924
0.420	6.7334	6.7036	6.6991	0.210	6.7334	6.3231	6.3228
0.440	6.7799	6.7601	6.7535	0.220	6.7799	6.4394	6.4391
0.460	6.8244	6.8133	6.8033	0.230	6.8244	6.5430	6.5426
0.480	6.8669	6.8644	6.8493	0.240	6.8669	6.6354	6.6349
0.500	6.9078	6.9078*	6.8919	0.250	6.9078	6.7178	6.7172
0.520	6.9470	6.9470*	6.9315**	0.260	6.9470	6.7916	6.7909
				0.270	6.9847	6.8578	6.8570
				0.280	7.0211	6.9176	6.9166
				0.290	7.0562	6.9719	6.9707
				0.300	7.0901	7.0215	7.0200
				0.310	7.1229	7.0672	7.0653
				0.320	7.1546	7.1094	7.1071
				0.330	7.1854	7.1489	7.1458
				0.340	7.2152	7.1859	7.1821
				0.350	7.2442	7.2210	7.2161
				0.360	7.2724	7.2545	7.2481
				0.370	7.2998	7.2867	7.2785
				0.380	7.3265	7.3179	7.3072
				0.390	7.3524	7.3485	7.3345
				0.400	7.3778	7.3778*	7.3604
				0.410	7.4025	7.4025*	7.3851**
* $\bar{U}(z)$		** $\bar{U}(z) - 0.0155$		* $\bar{U}(z)$		** $\bar{U}(z) - 0.0173$	

$K = 5000.0$				$K = 10000.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$	z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.	0.	0.	0.	0.	0.	0.	0.
0.010	4.6053	0.6118	0.6118	0.005	4.6053	0.4051	0.4050
0.020	5.2983	1.2187	1.2187	0.010	5.2983	0.8089	0.8089
0.030	5.7038	1.8157	1.8157	0.015	5.7038	1.2102	1.2102
0.040	5.9915	2.3981	2.3981	0.020	5.9915	1.6078	1.6078
0.050	6.2146	2.9610	2.9610	0.025	6.2146	2.0005	2.0005
0.060	6.3969	3.4999	3.4998	0.030	6.3969	2.3870	2.3870
0.070	6.5511	4.0105	4.0104	0.035	6.5511	2.7662	2.7662
0.080	6.6846	4.4889	4.4888	0.040	6.6846	3.1368	3.1368
0.090	6.8024	4.9318	4.9317	0.045	6.8024	3.4977	3.4977
0.100	6.9078	5.3367	5.3366	0.050	6.9078	3.8478	3.8477
0.110	7.0031	5.7021	5.7020	0.055	7.0031	4.1860	4.1859
0.120	7.0901	6.0276	6.0275	0.060	7.0901	4.5112	4.5111
0.130	7.1701	6.3139	6.3137	0.065	7.1701	4.8226	4.8225
0.140	7.2442	6.5629	6.5627	0.070	7.2442	5.1193	5.1192
0.150	7.3132	6.7774	6.7772	0.075	7.3132	5.4006	5.4005
0.160	7.3778	6.9607	6.9605	0.080	7.3778	5.6659	5.6658
0.170	7.4384	7.1169	7.1166	0.085	7.4384	5.9149	5.9148
0.180	7.4955	7.2496	7.2492	0.090	7.4955	6.1472	6.1472
0.190	7.5496	7.3626	7.3622	0.095	7.5496	6.3630	6.3629

TABLE II — *Concluded*

$K = 5000.0$				$K = 10000.0$			
z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$	z	$\bar{U}(z)$	$U_+(z)$	$U_-(z)$
0.200	7.6009	7.4595	7.4589	0.100	7.6009	6.5622	6.5621
0.210	7.6497	7.5431	7.5424	0.105	7.6497	6.7453	6.7452
0.220	7.6962	7.6161	7.6151	0.110	7.6962	6.9128	6.9126
0.230	7.7407	7.6805	7.6792	0.115	7.7407	7.0653	7.0652
0.240	7.7832	7.7382	7.7364	0.120	7.7832	7.2038	7.2036
0.250	7.8240	7.7907	7.7882	0.125	7.8240	7.3290	7.3289
0.260	7.8633	7.8390	7.8355	0.130	7.8633	7.4421	7.4419
0.270	7.9010	7.8841	7.8792	0.135	7.9010	7.5440	7.5438
0.280	7.9374	7.9270	7.9200	0.140	7.9374	7.6358	7.6355
0.290	7.9725	7.9685	7.9583	0.145	7.9725	7.7184	7.7181
0.300	8.0064	8.0064*	7.9947	0.150	8.0064	7.7929	7.7926
0.310	8.0392	8.0392*	8.0292	0.155	8.0392	7.8602	7.8598
0.320	8.0709	8.0709*	8.0623	1.160	8.0709	7.9212	7.9207
0.330	8.1017	8.1017*	8.0939	0.165	8.1017	7.9765	7.9760
0.340	8.1315	8.1315*	8.1243	0.170	8.1315	8.0270	8.0264
0.350	8.1605	8.1605*	8.1535**	0.175	8.1605	8.0733	8.0726
				0.180	8.1887	8.1159	8.1151
				0.185	8.2161	8.1554	8.1543
				0.190	8.2428	8.1921	8.1908
				0.195	8.2687	8.2265	8.2249
				0.200	8.2940	8.2589	8.2569
				0.205	8.3187	8.2896	8.2871
				0.210	8.3428	8.3187	8.3157
				0.215	8.3664	8.3466	8.3429
				0.220	8.3894	8.3735	8.3688
				0.225	8.4118	8.3995	8.3936
				0.230	8.4338	8.4248	8.4174
				0.235	8.4553	8.4496	8.4402
				0.240	8.4764	8.4740	8.4622
				0.245	8.4970	8.4970*	8.4833
				0.250	8.5172	8.5172*	8.5036**
* $\bar{U}(z)$		** $\bar{U}(z) - 0.0070$		* $\bar{U}(z)$		** $\bar{U}(z) - 0.0135$	

They have been rounded off and retabulated from the original IBM results, which were at shorter intervals and nominally to eight significant figures.

It goes without saying that one must be wary of roundoff and truncation errors when trying to integrate a stiff differential equation numerically. Even if one could start with exactly the right initial conditions, accumulated errors would shift the computation to a neighboring integral curve which would ultimately diverge rapidly from the desired solution. Strictly speaking, we cannot even be sure of the upper and lower bounds computed by stepwise integration of the differential equation, since roundoff errors could make two numerical solutions with nearly equal initial slopes cross each other and tend to infinity in the wrong directions. (No such crossing was observed in the present study.)

Unfortunately it is not easy, especially for the Runge-Kutta method, to obtain error bounds which are both rigorous and realistic. We therefore fell back on the usual test which is made to judge whether the error in a numerical integration is tolerable; namely, we ran the integration again with a double interval and compared results. This test was applied to most of the upper and lower bounds included in the tables. The difference between the two integrations was found to increase rapidly toward the end of the range, but always to be small compared to the difference between upper and lower bounds. In the worst case ($K = 0.1$) the difference between the two integrations for a given bound was less than one-tenth of the difference between upper and lower bounds; and for larger K the discrepancies were considerably smaller. We therefore feel quite confident that the tabulated results really are upper and lower bounds for the exact solution.

The range of the calculations shown here was chosen to bridge the gap between available approximations for small K (the "neutral" case) and large K (the "space-charge" case). For $K < 0.1$ the present method begins to run into instability trouble, though it could probably be modified to work for smaller values of K in the unlikely event that such calculations are wanted. For large K, on the other hand, there is no indication that $K = 10{,}000$ marks the upper limit of what can be handled with this technique.

In summary, then, a program has been written for the IBM 704 which will produce in a few minutes, for any value of K between 0.1 and somewhere above 10,000, very close upper and lower bounds for the potential distribution in a linearly graded p-n junction. A minor modification of the program would permit similar calculations for a junction with any reasonable distribution of fixed charge. So far as numerical techniques are concerned, therefore, the problem may be regarded as completely solved.

APPENDIX B

Numerical Capacitance Calculations

The neutral capacitance of a junction of normalized width z_l is given by (23) of the text as

$$C_n = \frac{C_0}{K^{\frac{1}{3}}}\left[I(z_l, K) - 3\frac{\partial I(z_l, K)}{\partial(\log K)} + z_l e^{-U_l}\right], \tag{B1}$$

where

$$I(z_l, K) = \int_0^{z_l} e^{-U(z,K)}\, dz. \tag{B2}$$

The value of I may be calculated numerically from Table II, which gives $U(z, K)$ for 16 values of K ranging from 0.1 to 10,000. Extension to arbitrarily large values of z_l is straightforward, since for sufficiently large z the tabulated functions differ by at most a constant from the asymptote $\bar{U}(z, K) = \sinh^{-1}Kz$. If U is replaced by $\bar{U} - \epsilon$ for $z \geqq z_0 \geqq 0$, where ϵ is constant, then provided that $z_l \geqq z_0$ and U is continuous at z_0, the expression for $I(z_l, K)$ becomes

$$I(z_l, K) = \int_0^{z_0} e^{-U} dz + \frac{e^{\epsilon}(U_l - U_0)}{2K} + \frac{z_l e^{-U_l} - z_0 e^{-U_0}}{2}. \quad \text{(B3)}$$

When K is small (the neutral case), then $U \approx \bar{U}$ for all z, and (B1) and (B3) yield the approximation (26).

The numerical evaluation of C_n/C_0 was carried out by evaluating $I(z_l, K)$ for each value of K using Simpson's rule. The function $\log I$ was then fitted at three adjacent values of K by a quadratic polynomial in $\log K$, and the derivative of I was found approximately by differentiating the polynomial at the middle value of K (except, of course, at $K = 0.1$ and $K = 10{,}000$, where the end value had to be used). The value of z_l was chosen to make $\bar{U}(z_l, K_1) = 10$, where K_1 is the point at which the derivative is evaluated. The value of z_l is supposed to be held constant during the differentiation.

Table III shows the values found for C_n/C_0 as a function of K. These values are actually averages of the results found by taking for $U(z, K)$ the upper and lower bounds given in Table II. The two numbers averaged differed from each other by less than 2 per cent in all cases, and usually by less than 1 per cent. As is well known, numerical differentia-

TABLE III — NORMALIZED CAPACITANCES

K	C_n/C_0	C_p/C_0
0.1	432	0.423
0.2	171	0.608
0.5	50.5	0.889
1	20.1	1.052
2	8.05	1.139
5	2.44	1.156
10	1.02	1.123
20	0.436	1.082
50	0.152	1.020
100	0.0721	0.972
200	0.0360	0.931
500	0.0153	0.883
1000	0.00834	0.850
2000	0.00468	0.822
5000	0.00225	0.790
10000	0.00132	0.762

tion magnifies the errors in inaccurate data. One may hope, however, that the values obtained for C_n are accurate to about 1 per cent. Comparison with the approximate formula (26) is shown in Fig. 6. Agreement is good for $K \lesssim 5$, but the approximation gives too low a value for C_n when K is large.

The space-charge capacitance is given by (24) as

$$C_p = \frac{C_0}{K^{\frac{1}{3}}}\left[3\frac{\partial S}{\partial(\log K)} - S\right], \tag{B4}$$

where

$$S = U'(0, K) \tag{B5}$$

is the initial slope of the potential function. The initial slope is given, as a function of K, to five significant figures in Table I. Logarithmic differentiation, using a three-point interpolating function, leads to the values of C_p/C_0 shown in Table III (the difference between the upper and lower bounds of the slope rarely affects the third decimal place). Again the accuracy is not precisely known, but is presumed to be 1 per cent or better.

For the neutral case, say $K \lesssim 0.2$, one has $S \approx K$ and

$$C_p \approx 2C_0K^{\frac{2}{3}}. \tag{B6}$$

When $K \gg 1$, the initial slope according to the space-charge approximation is

$$s = \left(\frac{3U_m \sinh U_m}{4}\right)^{\frac{1}{2}}, \tag{B7}$$

where U_m is defined in terms of K by (28). A straightforward if somewhat laborious substitution of (B7) and (28) into (B4) leads to

$$C_p = \frac{2(3U_m)^{\frac{1}{2}}C_0}{3U_m \coth U_m - 1}, \tag{B8}$$

as in (27). The approximation to C_p/C_0 given by (B8) is plotted against K in Fig. 6. It is seen that the approximate value of C_p lies above the correct value for K less than about 6, and below it, by amounts ranging up to nearly 10 per cent, for larger K.

REFERENCES

1. Shockley, W., Theory of p-n Junctions in Semiconductors and p-n Junction Transistors, B.S.T.J., **28**, 1949, p. 435; especially Section 2.
2. Moll, J. L., unpublished work.
3. Prim, R. C., unpublished work.
4. Morrison, J. A., unpublished work.
5. Kamke, E., *Differentialgleichungen*, 3rd ed., Chelsea, New York, 1948, p. 150.