CHARACTERISTICS OF TUNNELING P-N JUNCTIONS

by John B. Hopkins

Electronics Research Center
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SUMMARY

Procedures have been developed for the calculation of current-voltage characteristics of tunneling p-n junctions in semiconductors, given material constants and impurity-doping parameters. Accuracy higher than that acquired in similar efforts has been attained. When a digital computer is used, numerical differentiation permits calculation of parameters relevant to microwave mixing and detecting applications for tunnel and backward diodes in any elemental or compound semiconductor. Typical results are indicated.

INTRODUCTION

This report concerns research done in the fabrication and characterization of backward diodes made from a variety of III-V semiconductors. They are intended for use in microwave mixing and detecting applications. The research effort requires estimation of tunnel diode characteristics in a number of materials and for varying impurity concentrations. For example, it is useful to be able to estimate figures of merit which involve the first and second derivatives of the i-v curve, and these can be meaningful only with a fairly accurate knowledge of i(v). Determination of the theoretical i-v characteristics and other parameters of a p-n junction tunnel diode is a problem not amenable to an analytical approach.

A number of authors (refs. 1, 2, 3 and 4) have used greatly simplified models to obtain various numerical or analytical results, but—in addition to their very approximate nature—these solutions are limited in the information provided. This report describes results obtainable by use of an analysis significantly more detailed than that conventionally used. These calculations, facilitated by use of a digital computer, can be made to a significantly higher degree of accuracy than those previously reported.

It should be noted, however, that the calculations, though detailed, are ultimately based on the conventional physical model, and are therefore subject to errors resulting from the inadequacies of that representation. These weaknesses will be indicated at relevant points in the detailed description of the model and the calculations.
THE PHYSICAL MODEL

The model used is a conventional p-n junction. Perfect crystal structure is assumed, with an impurity concentration which changes abruptly from \( N_d \), at energy \(-E_d\) (n-region), to \( N_a \), at energy \( E_a \) (p-region). It should be noted that no real junction can be truly abrupt, and this assumption may well lead to inaccuracies when applied to tunneling junctions. For these, the "abruptness" condition (that the depletion layer be much wider than the region of changing impurity concentration) is seriously violated. Nor are defects of any type considered, so that this program does not show excess current. While this is a definite limitation for application to tunnel diodes (the peak-to-valley current ratio cannot be estimated, for example), it is forced by the theoretical complexity of the problem.

Further, it is of less relevance to backward diode studies, where operation is generally at very low bias, and excess current is small. The band structure is taken to be particularly simple—parabolic, and isotropic in \( \mathbf{k} \). Also, only direct tunneling transitions are considered. This could be a serious restriction, since both germanium and silicon are indirect-gap materials. However, the principal error will be only in current densities, so much useful information can be obtained for these materials as well. (Most III-V semiconductors of current interest are essentially direct-gap and accurate estimates can be obtained for them.)

Tunneling current is a very sensitive function of tunneling distance, and considerable care is taken in determining this parameter. The various material constants are specified for the temperature assumed, and are taken to be independent of applied voltage and Fermi levels, and as constant throughout the material. However, variation of the diffusion constant with the position of the Fermi level is included.

Discussion of tunnel diodes necessarily requires consideration of degenerate and near-degenerate conditions, and difficulties do arise—for example, in determination of the Fermi levels. Fortunately, some uncertainty in this does not seriously affect results in the region of principal interest. Further, an approximation has been developed which seems sufficiently accurate.

The required data for the material includes band gap, dielectric constant, lattice constant, and hole and electron mobilities, effective masses, and recombination times. The diffusion constants are calculated from the mobilities, using the Einstein relation \( D = kT \mu/q \), corrected for degeneracy. The diffusion lengths are determined from the diffusion constants and recombination times

\[
\ell = \sqrt{D \tau}
\]
In addition, the impurity doping parameters are read in. These include both concentrations and energy levels. Variation of mobility caused by increased impurity scattering for increasing doping density is incorporated by use of the Dingle-Brooks expression for impurity mobility.

As the program is intended to provide information about phenomena associated with low voltages only, no breakdown mechanisms have been included in the diode model.
DETAILS OF THE CALCULATIONS

The first step in determining the electrical characteristics of a semiconductor is calculation of the position of the Fermi level. For a p-n diode, this is done separately for the p and n regions. The basic equation used is that of charge neutrality:

\[
\text{[electrons in conduction band]} - \text{[holes in valence band]} - \text{[ionized donors]} + \text{[un-ionized acceptors]} = 0 \tag{1}
\]

The assumption is made that in the n region \(N_n = 0\), and in the p region \(N_d = 0\). (These restrictions could easily be removed, but have been made to avoid unnecessary complication of the program.) Through entirely conventional manipulations, equation (1) may be written:

\[
\int_0^\infty \frac{\epsilon^{1/2}}{1 + e^{\epsilon_f - \epsilon}} \frac{1}{K_e} \frac{1 - f_n(E_n)}{(kT)^{3/2}} - \frac{K_h}{K_e} \int_0^\infty \frac{\epsilon^{1/2}}{1 + e^{\epsilon_f - \epsilon_f + \epsilon}} \frac{1}{K_e} \frac{1}{1 + \exp(E - E_{f,n})} \, d\epsilon = 0 \tag{2}
\]

where

\[
\epsilon_f = E_f/kT, \quad \epsilon_g = E_g/kT
\]

\[
K_e = \frac{4\pi(2m_e)^{3/2}}{\hbar^2}, \quad K_h = \frac{4\pi(2m_h)^{3/2}}{\hbar^2}, \quad f_n(E) = \frac{1}{1 + \exp(E - E_{f,n})}.
\]

An analogous equation describes the p region. All three terms in equation (2) are functions of \(E_f\), and no closed analytic expression can be obtained. A simple iterative procedure is used (with a separate subroutine for the computer calculation) to determine the Fermi levels. For \(E_f\) less than \(-5\), the Ehrenberg approximation

\[
\left(\text{Fermi integral} = 2\pi^{1/2} \frac{e^{\epsilon_f}}{1 + \epsilon_f} \right)
\]

is used; otherwise numerical integration is carried out with increments of 0.1 over the range from zero to

\[
\left[25 + \epsilon_f^2\right]^{1/2}.
\]

(A change of variable \(u = \epsilon_f^{1/2}\) is made to cause the integrand to vanish more quickly.) The iteration for \(E_f\) consists of successive halving of an interval originally chosen to include the expected value. Any desired accuracy can be obtained; the value used for the uncertainty in \(E_f\) is 0.01 (.00026 eV).

When calculations of \(E_f\) for the n and p regions have been made, carrier concentrations are immediately determined from
where

\[ \epsilon_i = E_g / kT, \quad \eta_c = \frac{E_f - E_c}{kT}, \quad \eta_v = \frac{E_f - E_v}{kT}, \quad \]

and

\[ F_{1/2}(\epsilon) = \int_0^\infty \frac{x^{1/2} \, dx}{1 + \exp(x - \epsilon)} \]

If the material mobility is known, conductivity may then be calculated as

\[ \sigma = n q \mu_e + p q \mu_h . \]

Degeneracy (impurity concentrations such that the Fermi levels are within the n-region conduction band and the p-region valence band) presents some difficulty. At these impurity concentrations, the assumption that all impurities are at a particular energy level, with no interaction, is significantly in error. The theoretical situation is quite involved, and no simple, generally valid result is available. However, at this point the dependence of device characteristics becomes somewhat less critical. An empirical approximation -- \( f(E_f) = 1/3 \) for \( E_f \) above the donor level or below the acceptor level -- seems to agree fairly well with relevant published data (e.g., ref. 4). (This gives a continuous function, since \( f_n(E_c) = f_p(E_v) = 1/3 \).) Such an approximation is unlikely to be accurate at strong degeneracy, but that is a situation rarely found. For backward diodes (the principal subject of this study) only slight degeneracy occurs. Mobility is affected markedly by high impurity concentrations, and a correction is necessary. The one chosen is that of Dingle and Brooks (refs. 5, 6), for which the mobility \( \mu_I \) caused by impurity scattering is given by

\[ \mu_I = \frac{64 \pi^{1/2} \epsilon^2 (2kT)^{3/2}}{N_I Z^2 e^3 m_e^{1/2}} \left[ \ln \left( \frac{24 m_e k^2 T^2 \epsilon}{e^2 h^2 N_I} \right) \right] \]

and the total mobility is taken as

\[ \mu = \frac{\mu_o \mu_I}{\mu_o + \mu_I} \]

with \( \mu_o \) the mobility at low doping, caused principally by lattice scattering.
One further correction for degenerate circumstances involves the diffusion constants, which are also somewhat affected by heavy doping. Again a small empirical correction is made: \( D = (1 + 2 E_f) D_0 \) within the conduction and valence bands, where \( D_0 \) is the value at low doping.

The next step is computation of device behavior under applied bias. All voltage drop is assumed to take place across the junction, and -- following generation of the specified applied voltages -- the thickness and shape of the depletion region are determined. Again, this is a conventional calculation, based on the assumption of an abrupt junction, and is outlined in Appendix I. Junction capacitance (per unit area) is then calculated from the depletion layer width and the dielectric constant of the material. For a specified junction area, junction (barrier) capacitance \( C_B \) is then known, as is the spreading resistance, \( R_S \), which is determined from the semiconductor conductivity: \( R_S = 1/4 \sigma r \), where \( r \) is the junction radius.

As indicated in Appendix I, the actual tunneling distance is different from the junction width, though related to it, and this is used in the next section where tunnel current is calculated.

The tunnel current across a p-n junction is generally given by

\[
I_t = \int_{E_c}^{E_v} \rho_c(E) \rho_v(E) f_n(E) \left[ 1 - f_r(E) \right] P_t \, dE, \quad E_v \geq E_c
\]

\[
= 0, \quad E_{vp} \leq E_{cn}
\]  

(3)

The tunneling probability \( P_t \) is calculated from quantum mechanics, with a triangular energy barrier assumed, and is usually taken as

\[
P_t = A \frac{a q}{\hbar} \bar{F} \exp \left\{ - \frac{\pi^2}{2} \left( \frac{2m*q}{\hbar} \right) \right\}
\]

(4)

where \( \bar{F} \), the average field across the junction, is taken as

\[
\bar{F} = \frac{q}{E} \left( d_p - \frac{t}{2} \right) \frac{N_a N_d}{N_a + N_d}
\]

with the tunneling distance \( t = t(E) \), as given in Appendix I.

The numerical integration (according to Simpson's rule) is carried out by dividing the energy interval into 20 parts, which is found to give results not significantly different from division into 100 parts. As indicated before, the energy bands are assumed to be parabolic, so
\[ \rho_c(E) \propto (E - E_c)^2 \]

and

\[ \rho_v(E) \propto (E_v - E)^2 \]

within the bands and zero elsewhere.

For reference, the normal diode current is also calculated. This is given by

\[ I = I_s \left[ \exp \left( \frac{q V_{ap}}{kT} \right) - 1 \right] \]  \hspace{1cm} (5)

with \( I_s \) determined from carrier concentrations, and diffusion constants and lengths:

\[ I_s = q \left[ \frac{D_n n_0}{L_n} + \frac{D_p p_0}{L_p} \right] . \]

The validity of this result is somewhat limited, as diffusion lengths are seldom known with any precision, and, in addition, other mechanisms often add considerably to this current. However, it is generally not very significant in the region of interest (low applied voltages), particularly when substantial tunneling occurs.

The peak voltage is determined by a simple iterative scheme. Tunnel current is calculated for increasing values of voltage until two successive currents show a decrease. The procedure then repeats from the last increasing point, with a reduced voltage increment. After several such cycles, an accuracy of better than 0.1 mV can be obtained. Thus, for each specified value of applied voltage, the program calculates resulting tunnel current, diffusion current, junction width and capacitance, and "average" tunneling distance (see Appendix I). The value of current associated with peak voltage is then used to normalize the tunnel current values. In addition, useful information concerning device properties can be obtained from the first and second derivatives of the current-voltage characteristic. For example, current sensitivity \( \beta_0 \) is given by \( f''/f \) where \( i = f(v) \). Numerical differentiation is difficult to accomplish with significant accuracy, particularly for higher derivatives. The method used here involves calculation of current-voltage data points displaced from the point of interest by plus-and-minus 1- and 2-volt increments. These are used (as shown in Appendix II) to approximate \( f'(v) \) and \( f''(v) \). The size of the voltage increment to be used must be a compromise, as the natural choice of a small increment results in a set of data points so close together that differences between them become very small, and even the eight-place accuracy of a computer is inadequate. The optimum size has been determined by comparison of different trials, taking as a criterion that variation should be smooth from point to point. An increment of 1 mV has proven satisfactory and should prove compatible with experimental techniques.
The physical model used does not permit determination of actual currents or current densities with meaningful accuracy. However, published experimental data can be used to obtain approximate calibration constants to relate the calculated values to actual currents. With these estimates, the barrier resistance $R_B (1/f')$ is easily calculated, and with the capacitance $C_B$ and spreading resistance $R_S$ obtained previously -- a number of figures of merit useful for microwave device characterization can be found:

$$\beta_0 = f''/f'$$

$$f_c = \frac{[1 + (R_S/R_B)]^{1/2}}{2\pi C_B (R_S R_B)^{1/2}}$$

$$\beta(f_o) = \beta_0 \frac{1}{(1 + R_S/R_B) [1 + (f_o/f_c)^2]}$$

$$M = \beta R_B^{1/2}$$

Running time on a digital computer for these calculations can be quite short. On a Univac 1108, compilation requires 4 seconds, and the determination of Fermi levels, carrier concentrations, peak voltage and current, and so forth, takes approximately 0.5 second. Several hundred i-v data points may be calculated in 1 second.
SUMMARY AND CONCLUSIONS

The calculations described above may be thought of as comprising two major parts -- computation of Fermi levels, and determination of resulting material and diode parameters. The accuracy of the Fermi level calculation is difficult to check, but agrees fairly well with published estimates. One check is comparison with the data compiled by Irvin (ref. 7) showing resistivity versus doping for n-type silicon. His values represent an averaging of published experimental data, with 90 percent of the actual points falling within 10 percent of his curve (below \( N_d = 10^{19} \)). The match of calculated resistivity with Irvin's curve is shown in Figure 1, and is quite good up to \( 5 \times 10^{20} \), at which point impurity scattering and conduction produce a situation too complex to treat usefully in any simple fashion.

Typical calculations of Fermi level as a function of impurity concentration, near the band edge, are shown in Figure 2. The current-voltage characteristics for a particular diode is graphed in Figure 3 where two calculated curves are compared to measured values for a GaSb unit. One calculation is simply

\[
\int_{E_c}^{E_v} \rho_c(E) \rho_v(E) f_n(E) [1 - f_p(E)] dE
\]

as used by Esaki (ref. 4) and others, and for which a good numerical approximation has been developed by Bates (ref. 8). The other computation includes the tunneling distance and probability as variables within the integral. The latter approach is seen to offer substantially higher accuracy, matching quite well until excess current, probably associated with tunneling between impurity states, becomes significant. \( (N_d \text{ and } N_a \text{ were chosen in each case to match the peak voltage of the experimental curve.}) \)

Figures 4 and 5 are typical computer printouts. Figure 4 illustrates simple i-v curve data, while Figure 5 is a sample of the figure of merit calculations.

The calculations that have been described are not presented as an exact solution of high accuracy. Indeed, many approximations and weaknesses have been indicated. However, computations based on this model have been found to be of use, providing significant improvement over the simpler approaches generally taken in articles and textbooks to obtain estimates of both numerical values and the relation between different variables. For example, the improvement in determination of current-voltage characteristics should make possible meaningful comparison of various semiconductors in terms of their suitability for fabrication of backward diodes to be used for microwave detection and mixing. Further, useful information can be obtained concerning optimum doping and performance as a function of temperature.
Figure 1. -- Resistivity versus impurity concentration for n-type silicon (comparison of computer results and those of Irvin, BSTJ, vol. 41, p. 387, 1957.)

Figure 2. -- Degeneracy versus impurity concentration - InAs
In summary, this formulation permits rapid and easy estimation of approximate device characteristics, with significantly better accuracy than has been possible with previous simpler approaches.

Figure 3. --Comparison of calculated and experimental tunnel diode characteristics (GaSb) (matched for peak current and voltage; equal degeneracy for both bands)
GERMANIUM

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<th>MU(P)</th>
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DiELECTRIC CONSTANT = 16.00
LATTICE CONSTANT = 5.66 ANGSTROMS

Temp (K.) = 300.0
JUNCTION AREA = 2.50 x 2.50 MICRONS = .625-07 SQ. CM.
MOBILITY(IMPURITY) N = 534, P = 360.

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MOBILITY (IMPURITY) = N = 534, P = 360

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<td>.1400</td>
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<td></td>
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</table>

Figure 4. --Simple i-v curve data
GERMANIUM

\[
\begin{align*}
E(G) &= .07 \\
M(E) &= .22 \\
M(H) &= .38 \\
M(U(N)) &= 3800.00 \\
M(U(P)) &= 1800.00 \\
D(N) &= 94.22 \\
D(P) &= 40.53 \\
L(N) &= 70.33 \\
L(P) &= 41.43 \\
T(N) &= .50-03 \\
T(P) &= .50-03 \\
\text{DIELECTRIC CONSTANT} &= 16.00 \\
\text{LATTICE CONSTANT} &= 5.66 \text{ ANGSTROMS}
\end{align*}
\]

\[
\begin{align*}
\text{TEMP (K.)} &= 300.0 \\
\text{JUNCTION AREA} &= 10.00 \times 10.00 \text{ MICRONS} = .100-05 \text{ SQ. CM.} \\
\text{MOBILITY (IMPURITY) N} &= 534. \\
\text{P} &= 360. \\
\text{D(N)} &= 8.22 \\
\text{D(P)} &= 40.53 \\
\text{L(N)} &= 70.33 \\
\text{L(P)} &= 41.43 \\
\text{T(N)} &= .50-03 \\
\text{T(P)} &= .50-03 \\
\text{FERMI FUNCTION FROZEN AT EC(N)} &= -.030 \\
\text{EC(P)} &= .030 \\
\text{PEAK CURRENT} &= .1683-03 \\
\text{PEAK VOLTAGE} &= 50.58 \text{ MV.} \\
\text{BAND OVERLAP} &= 199.7 \text{ MV.} \\
\text{IC/CJ} &= .084973657 \\
\text{NO(N)} &= .20+20 \\
\text{NO(P)} &= .20+20 \\
\text{PO(N)} &= .20+20 \\
\text{PO(P)} &= .20+20 \\
\text{RHO(N)} &= .584-03 \text{ OHM-CM.} \\
\text{RHO(P)} &= .869-03 \text{ OHM-CM.} \\
\text{RS(N)} &= .259 \text{ OHMS} \\
\text{RS(P)} &= .385 \text{ OHMS}
\end{align*}
\]

<table>
<thead>
<tr>
<th>VOLTAGE (MV)</th>
<th>CURRENT (OHMS)</th>
<th>FIG OF MERIT</th>
<th>RB (OHMS)</th>
<th>FC (GZH)</th>
<th>TUN. DIST. (ANG)</th>
<th>CAP. (PF)</th>
<th>1</th>
<th>2</th>
<th>5</th>
<th>10</th>
<th>20</th>
<th>50</th>
<th>100</th>
<th>M</th>
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<td>6.5</td>
<td>7.6</td>
<td>6.0</td>
<td>9.0</td>
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<tr>
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<td>10.05</td>
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<td>6.5</td>
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<td>9.0</td>
<td>4.9</td>
<td>65.65</td>
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<td>5.7</td>
<td>6.5</td>
<td>7.6</td>
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<td>9.0</td>
<td>4.9</td>
<td>65.65</td>
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</table>

Figure 5. -- Figure of merit calculations
REFERENCES


The quantities necessary for the determination of depletion layer and tunneling thickness are indicated in Figure A-1. The zero of potential is taken as the bottom of the n-region conduction band, far from the junction. The doping is assumed to change abruptly from \( N_d \) (n region) to \( N_a \) (p region) at \( x = 0 \). It is convenient to define \( V_n(x) \) and \( V_p(x) \) as the potential

\[
V_p(x) = -\frac{qN_a}{\epsilon} \left( \frac{x^2}{2} + d_p x \right) + V_o' \quad \text{for} \quad d_p < x < 0
\]

\[
V_n(x) = \frac{qN_d}{\epsilon} \left( \frac{x^2}{2} - d_n x \right) + V_o'' \quad \text{for} \quad 0 < x < d_n
\]
The terms \( d_p \) and \( d_n \) represent the x-values for which space charge (and therefore the electric field) is taken as zero. This condition defines the boundaries of the depletion region. \( V'_{o} \) and \( V''_{o} \) are integration constants and must be equal, since \( V_{p}(0) = V_{n}(0) = V'_{o} = V''_{o} \). Further

\[
V_n(d_n) = q \frac{N_d}{\epsilon} \left( -\frac{d_n^2}{2} \right) + V'_{o} = 0 ,
\]

so

\[
V'_{o} = V''_{o} = V_{o} = q \frac{N_d}{\epsilon} \frac{d_n^2}{2}
\]

From Figure A-1, it can be seen that

\[
V_{p}(-d_p) = E_g + \delta v_n - \delta v_p - \nu_{ap} = E_g + \delta v
\]

or

\[
q \frac{N_a}{\epsilon} \frac{d_p^2}{2} + q \frac{N_d}{\epsilon} \frac{d_n^2}{2} = E_g + \delta v .
\]

An equal amount of (space) charge must exist on either side of the junction, so that

\[
q N_d d_n = q N_a d_p
\]

or

\[
d_n = \frac{N_a}{N_d} d_p
\]

So:

\[
q \frac{N_a}{\epsilon} \frac{d_p^2}{2} + q \frac{N_d}{\epsilon} \frac{1}{2} \cdot \left( \frac{N_a}{N_d} d_p \right)^2 = E_g + \delta v
\]

\[
\frac{d_p^2}{q} \left( \frac{q N_a^2}{2 \epsilon} + \frac{q N_d^2}{2 \epsilon N_d} \right) = E_g + \delta v
\]
and

\[ d_p = \sqrt{\frac{2\varepsilon}{q} \left( \frac{E_g + \delta\nu}{N_a N_d + N_d^2} \right) N_d} \]

\[ d_n = \sqrt{\frac{2\varepsilon}{q} \left( \frac{E_g + \delta\nu}{N_a N_d + N_d^2} \right) N_a} \]

with the total width of the depletion region \( d = d_n + d_p \), and the junction capacitance \( C = A\varepsilon/d \).

The tunneling distance, for carriers of a particular energy, is \( x_n - x_p \), with \( x_p \) generally negative. This distance exists only in the range \( \delta\nu > 0 \).

For \( d_p < x < 0 \), the expression for the top of the p-region valence band is:

\[ V_p(x) - E_g = \frac{qN_a}{\varepsilon} \left( x^2 + d_p x \right) + q \frac{N_d}{\varepsilon} \frac{d^2}{2} - E_g, \]

and for the bottom of the n-region conduction band:

\[ V_n(x) = \frac{N_d}{\varepsilon} \left( \frac{x^2}{2} - d_n x \right) + q \frac{N_d}{\varepsilon} \frac{d^2}{2}. \]

For \( \delta\nu_0 \), a particular value of \( V \), with \( 0 < \delta\nu_0 < \delta\nu \), \( x_n \) and \( x_p \) are implicitly determined from

\[ V_p(x) - E_g = \delta\nu_0 = -q \frac{N_a}{\varepsilon} \left( \frac{x_p^2}{2} + d_p x + \frac{N_d d_n^2}{N_a} \right) - E_g \]

and

\[ \delta\nu_0 = q \frac{N_a}{\varepsilon} \left( \frac{x^2}{2} - d_n x + \frac{d_n^2}{2} \right), \]
or rewriting:

\[
\frac{x_p^2}{2} + d_p x_p + \left[ \frac{\epsilon}{qN_a} (E_g + \delta v_o) - \frac{N_d}{N_a} d_n^2 \right] = 0
\]

\[
\frac{x_n^2}{2} - d_n x_n + \left[ -qN_d - \delta v_o + \frac{d_n^2}{2} \right]
\]

so

\[
x_p = -d_p + \sqrt{\frac{d_p^2}{2} + \left[ \frac{N_d}{N_a} d_n^2 - \frac{2\epsilon}{qN_a} (E_g + \delta v_o) \right]}
\]

\[
x_n = d_n - \sqrt{\frac{2\epsilon}{qN_d} \delta v_o} \quad 0 < \delta v_o < \delta v
\]

(The correct signs for the radicals are determined by consideration of limiting cases.) Thus:

\[
t = d_n - (-d_p) - \sqrt{\frac{d_p^2}{2} + \frac{N_d}{N_a} d_n^2 - \frac{2\epsilon}{qN_a} (E_g + \delta v_o)} - \sqrt{\frac{2\epsilon}{qN_d} \delta v_o}
\]

\[
= d - \sqrt{\frac{d_p^2}{2} + \frac{N_d}{N_a} d_n^2 - \frac{2\epsilon}{qN_a} (E_g + \delta v_o)} - \sqrt{\frac{2\epsilon}{qN_d} \delta v_o}
\]

For specified materials and doping, the degeneracy (\(\delta v_p\) and \(\delta v_n\)) is known, and \(\delta v\) is linearly related to the applied voltage. To calculate the tunnel current, one can now integrate over \(V\) from zero to \(\delta v\), with tunnel distance \(t\) being a known function of potential. An "average" tunnel distance can also be determined. This quantity is somewhat arbitrary; in this program it is defined by

\[
\overline{t} = \frac{1}{\delta v} \int_0^{\delta v} t(v) \, dv.
\]
APPENDIX I

NUMERICAL DETERMINATION OF FIRST AND SECOND DERIVATIVES

Consider a function \( f(x) \), known at a set of equally spaced points \( x_{-k}, x_{-(k-1)}, \ldots x_1, x_0, x_1, \ldots x_k \), with \( f_k = f(x_k) \). One can define "central differences" of various order as follows:

\[
\delta f_0 = \frac{1}{2} (f_1 - f_{-1})
\]

\[
\delta^2 f_0 = \frac{1}{2} \left( \delta f_1 - \delta f_{-1} \right) = f_1 - 2f_0 + f_{-1}
\]

\[
\delta^3 f_0 = \frac{1}{2} \left( \delta^2 f_1 - \delta^2 f_{-1} \right) = \frac{1}{2} (f_2 - f_{-2}) - (f_1 - f_{-1})
\]

\[
\delta^4 f_0 = \frac{1}{2} \left( \delta^3 f_1 - \delta^3 f_{-1} \right) = 6f_0 - 4f_1 - 4f_{-1} + f_2 + f_{-2}
\]

As shown in standard references on numerical analysis (ref. II-1), the first and second derivatives of \( f \), evaluated at \( x_0 \), are then given by

\[
f'_0 = \frac{1}{h} \left( \delta f_0 - \frac{1}{6} \delta^3 f_0 \right) + \text{terms of higher order}
\]

\[
f''_0 = \frac{1}{h^2} \left( \delta^2 f_0 - \frac{1}{12} \delta^4 f_0 \right) + \text{terms of higher order}
\]

with \( h = x_k - x_{k-1} \).

These expressions are used in the diode computer program, with \( h = 1 \) mV.

Electronics Research Center
National Aeronautics and Space Administration
Cambridge, Massachusetts, November 1967
125-21-03-11

"The aeronautical and space activities of the United States shall be conducted so as to contribute . . . to the expansion of human knowledge of phenomena in the atmosphere and space. The Administration shall provide for the widest practicable and appropriate dissemination of information concerning its activities and the results thereof."

—NATIONAL AERONAUTICS AND SPACE ACT OF 1958

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