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Cheng, Li-Pin Bill

IMPURITY BAND FORMATION BY SCREENED INTERACTIONS OF NEIGHBORING IMPURITIES IN SEMICONDUCTORS

The Ohio State University

Ph.D. 1965

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IMPURITY BAND FORMATION BY SCREENED INTERACTIONS
OF NEIGHBORING IMPURITIES IN SEMICONDUCTORS

DISSERTATION

Presented in Partial Fulfillment of the Requirements for
the Degree Doctor of Philosophy in the Graduate
School of the Ohio State University

By

Li-Pin B. Cheng, B.S., M.S.

The Ohio State University

1985

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According to V. L. Bonch-Bruyevich\textsuperscript{1}, one of the pioneers in the subject of heavily doped semiconductors, as a consequence of the discovery of the tunnel diode the study of electronic properties in materials containing a relatively large concentration of impurity atoms has become of primary importance (V. I. Fistul\textsuperscript{2}). However, the area of application of heavily doped materials is actually much broader. These semiconductors are used in, among other devices, lasers, thermoelectric devices, photo-voltaic devices, semiconductor catalysts and thin films.

One result of the miniaturization of semiconductor devices is the increase in doping levels of semiconductors. As Keyes\textsuperscript{3} pointed out, a basic reason for this is the limitation placed on transistor dimensions by depletion layers. The electric fields produced by the charge of the fixed donors or acceptors must support the potential difference between the n and p regions of a junction. The greater the charge density or doping level, the greater the electric fields, and the thinner the depletion layer needed to accommodate the potential difference, thus, an increase in doping level is needed to accompany miniaturization.

The term impurity should not necessarily be interpreted literally — it can refer to any structural point defect that leads to
a disturbance of strict periodicity of the lattice. Obviously the study of heavily doped semiconductors is a part of the more general problem of disordered structures, the study of this subject has generated considerable activity in solid state physics, both theoretical and experimental.

It is well known that isolated impurity atoms can lead to the creation of discrete levels located in the forbidden band. The wave function of an electron occupying such a level is localized in the vicinity of the impurity atom. When the impurity concentration is increased, wave functions of the associated electrons begin to overlap. Under such conditions, the impurity energy levels should become perturbed in the same way as do the levels of the atoms of a crystal relative to their discrete nature in the vapor phase. A complete band of allowed states appears in the forbidden band. It is commonly called the impurity band. The case where the impurity band is separated from an intrinsic band by a forbidden region can be designated as a moderately doped semiconductor.

The impurity concentration at which an impurity band becomes noticeably wide, and conductive, can be determined experimentally. When an impurity band exists and is sufficiently wide, the electrical conductivity does not become zero upon freezing out electrons from the conduction band by lowering the temperature, but remains finite, though small (Mott \(^4\)). The width of the impurity band obviously increases as impurity concentration is increased. At a sufficiently high impurity concentration \(C\), the activation energy for promoting a localized electron to the conduction band finally becomes zero. In
silicon doped with group V donors, this occurs at $C \approx 10^{18} \text{ cm}^{-3}$ (Pearson$^5$, Fritzsch$^6$). This would indicate that the upper edge of the impurity band reaches into the conduction band. Under this condition, the semiconductor can be designated as being heavily doped.

Bonch-Bruyevich$^7,8$ studied lightly doped semiconductors under high electron injection conditions. The donor level is moved toward the conduction band because of screening of the field of the donor atoms by the injected free electrons. This applies particularly to shallow donors whose fields are of longer range and are more readily affected by shifts in the free electron concentration. As the injection level is increased, the ground state level of the localized electron is moved closer and closer to the conduction band, and finally disappears. If screening is to reduce the range of the field of an ionized donor to $r$, then it is evident that the disappearance of the levels takes place when $r$ becomes comparable to the first Bohr radius in the crystal. For silicon, the concentration of free electrons at which this occurs is about $10^{18} \text{ cm}^{-3}$. This is just the concentration that characterizes a heavily doped silicon. Therefore screening plays an important role in heavily doped semiconductors where free charge carriers are supplied by the impurities. If, however, it is assumed that all the electrons are localized, then there will in general be no free charges, and hence no screening. This means that the problem demands a self-consistent approach, the energy spectrum depends on the distribution of charge carriers,
which, in turn, is itself determined by the form of the energy spectrum of the semiconductor.

G. D. Mahan and K. F. Berggren used a nearly-free electron approximation to calculate the band gap narrowing in heavily doped n-Si and Ge as a function of impurity concentration at \( T = 0 \) K. For impurity concentration \( C \), the average kinetic energy of the conduction band electrons is of the order \( \hbar^2 C^{2/3}/2m \), while the interaction energy between electrons is of the order \( e^2 C^{1/3}/\epsilon \), where \( \epsilon \) is the crystal dielectric constant. The ratio of kinetic energy to interaction energy is therefore of the order \( C^{1/3}(\epsilon \hbar^2/m \epsilon) \) or \( C^{1/3} a \), where \( a \) is the Bohr radius. The nearly-free electron approximation is plausible for \( C^{1/3} a \geq 1 \) or \( C \geq 10^2 \) cm\(^{-3}\) for Si or Ge. This can also be understood from the fact that, since \( C^{-1/3} \) is comparable to the average distance between neighboring impurity atoms, \( C^{1/3} a \) is therefore comparable to the ratio of the Bohr radius to the average interimpurity distance. The relation \( C^{1/3} a \sim 1 \) means that there is substantial overlapping among electron wave functions, therefore the electrons are nearly free in the sense that they are highly delocalized. Mahan used a variational method in his calculation, while Berggren used a perturbation method. Their results are in general agreement with each other.

M. Balkanski and P. E. Schmid measured the band gap narrowing in heavily doped n-Si using an optical method. H. P. D. Lanyon and A. Neugroschel used an electronic device method in their measurements. A compilation of both theoretical and experimental results showed an order of magnitude agreement with one another.
However, there is a considerable numerical disagreement. This is due to the approximations in various theoretical approaches and the inaccuracy in interpretation of experimental data. Part of the confusion is caused by the Burstein-Moss\textsuperscript{15,16} effect. This is because the Fermi level could move above the bottom of the conduction band as the doping level is increased. Therefore, the lowest energy transition in optical absorption is not to the bottom of the conduction band, but to the Fermi level. For this reason, it is necessary to specify carefully what is meant by the top of the band gap. The energy gap of the doped semiconductor is different from that of the undoped semiconductor by yet another quantity. This is because the energy gap is defined as the minimum energy required to make an electron-hole pair in the semiconductor. Therefore, the hole's self energy which arises from the potential energy with the electrons and with the screened donors has to be taken into account (Mahan\textsuperscript{9}, Berggren\textsuperscript{10}). Another difficulty is due to the randomness of impurity sites with the result that band edges are not sharp. This is called band tailing (Abram\textsuperscript{17}).

On the other hand, for dilute systems, inter-impurity distance $C^{-1/3}$ is large compared with Bohr radius $a$. The electron wave functions are essentially isolated under this condition, namely $C^{1/3} a \ll 1$. W. Y. Ching\textsuperscript{18} calculated energy spectrum in these systems using tight binding approximation.

B. I. Shklovskii\textsuperscript{19} studied electric conduction in lightly doped semiconductors at temperatures sufficiently low that nearly all charge carriers are frozen out. The conduction under this condition
is mainly due to electrons hopping from occupied donors to empty ones without any excursion to the conduction band, called hopping conduction. The presence of empty donors is caused by compensation, and the electron jumps are associated with a weak overlap of wave-function tails from neighboring donors. Hopping conduction was theoretically predicted by Gudden and Schottky, and the first experimental data on it were obtained by Bush and Labhart for silicon carbide and by Hung and Gliessman for silicon and germanium. For Ge, it occurs at $T \sim 7$ K for donor concentration $C \sim 10^{15} \text{ cm}^{-3}$. For higher impurity concentration, the impurity band broadens and the system goes into a metallic state as the Mott transition ($\text{Mott}^{23, \text{Khomskii}^{24}}$) occurs.

Shklovskii also studied very heavily doped semiconductors, namely $C^{1/3} a \gg 1$. As explained earlier, this condition implies that the electron kinetic energy is large compared with potential energy. Therefore, the electron gas resembles an ideal gas. Bonch-Bruyevich, Kane, and Keldysh calculated the density of states for these systems using a semiclassical picture. Due to the randomness of impurity sites, the density of states has a tail region that extends into the forbidden gap. Halperin and Lax, Zittartz and Langer, and I. M. Lifshitz proposed a method to determine the density of states in its tail region.

One objection to the results obtained in theoretical works described above is that neither the tight-binding approximation nor the nearly-free electron approximation applies well in the range
$C^{1/3}a \lesssim 1$, which is of great practical interest. Another objection is the practice of assuming that the impurity atoms are located in a regular lattice rather than in a random arrangement. Furthermore, the same can be said of the practice of setting temperature at 0 K rather than over a wider range of interest. The purpose of the present work is to incorporate the effects of free carrier screening and interactions between randomly placed impurities over wide ranges of temperature and impurity concentration in order to reveal the results of these effects. A simple model separating impurities into pairs is used for this purpose. I. M. Lifshitz$^{33}$ first studied in detail this model which pairs up each impurity atom with its nearest neighbor and ignores interactions beyond the pair level. In the present work, this model is extended to include the screening effect. It can be justified as providing a good approximation to screening effects as well as a useful indication of neighbor interaction effects, partly because of the pairing habits of electrons and partly because the screening limits the impurity interaction range. It can be shown to give good results over a wide range of impurity concentrations and temperatures. Ground state energies of localized electrons in a donor pair are calculated. These results are used to calculate Fermi energy and density of states.
II. THEORY

In the present work, semiconductors are assumed to be n type to simplify terminology, however, with proper changes in interpretation, the results apply to p type semiconductors as well. At low donor concentration, the problem of the isolated shallow donor has been thoroughly explored, both theoretically (W. Kohn, R. A. Faulkner) and experimentally (P. Fisher). It is established that the localized electron wave function is hydrogen-atom like, as evidenced by the optical absorption spectrum which consists of sharp lines forming a hydrogen like series (P. Fisher). At higher donor densities, the overlapping between neighboring localized electron wave functions makes it necessary to calculate the interactions between the two electrons. The effect of the free charge carriers is accounted for by screening the field of the ionized donors and localized electrons. Following common practice, the effect of the host crystal is accounted for by modifying the electron mass and the dielectric constant.

From a pair of donors, the energy needed to ionize two localized electrons is denoted as $E_{12}$. The energy needed to ionize a single localized electron from the pair of donors is denoted as $E_1$. Then $E_2$ where $E_2 = E_{12} - E_1$, is the energy needed to ionize one of two localized electrons from the donor pair.
1. Calculation of $E_1$ and $E_2$

Let $R$ be the distance between donor atoms. Using linear approximation in classical screening theory (Schklovskii\textsuperscript{19}), let $B$ be the screening factor. Then the screening factor is

$$B = \left( \frac{q^2}{\varepsilon kT} \frac{dn}{dn_f} \right)^{1/2} \quad (2-1)$$

where $\varepsilon$ is the dielectric constant, $n$ is free charge carrier concentration, and $n_f$ is Fermi energy divided by $kT$.

The screened potential energy magnitude has the form

$$V_{ij} = 2 \exp(-8ri_j)/ri_j \quad (2-2)$$

With energies in units of Rydbergs and distances in units of Bohr radii, the Hamiltonian operator for two electrons bound to a pair of impurity ions has the form

$$H = -V_1^2 - V_2^2 - V_{1a} - V_{1b} - V_{2a} - V_{2b} + V_{12} \quad (2-3)$$

The impurity ions are located at points a and b separated by a distance $R$. Distances from these centers to electrons at points 1 and 2 are denoted by $r_{1a}$, $r_{1b}$, $r_{2a}$, and $r_{2b}$. The inter-electron distance is $r_{12}$. Two angles $\phi_1$ and $\theta_2$ locate the azimuthal positions (Fig 2.1). The ground state wave function for the system is constructed from basis functions of the form

$$a(1) = (a^3/n)^{1/2} \exp(-ar_{1a}) \quad (2-4)$$

where $a(1)$ is the $1s$ wave function for electron 1 at impurity site $a$. Similar $1s$ wave functions are formed for electron 1 at impurity
Figure 2.1: Relative positions of impurity ions and electrons.
site b, electron 2 at impurity sites a and b. The normalized
ground state wave function is of the form

\[ \psi_U = (2(1 + s^2))^{-1/2} [a(1)b(2) + a(2)b(1)]U_A \]  \hspace{1cm} (2-5)

where \( U_A \) is an antisymmetric spin function and \( S = \int a(1)b(1)dv_1 \)
is the overlap integral. The quantity \( \alpha \) in the basis 1s function
is the variational parameter and for an isolated hydrogen-like
atom it takes the value unity when distances are in Bohr radii.

The expectation value of \( H \) is computed for each value of
impurity separation, \( R \), and for the screening parameter, \( \beta \),
by minimizing the energy with variation in \( \alpha \). Since the Hamil-
tonian is spin-independent, it is possible to compute its expec-
tation value without considering spins. The positive sign in
the wave function \( \psi \) is associated with a symmetric function of
co-ordinates and produces the singlet state which is the ground
state.

Integrals that are needed for the energy calculations come
from the expression

\[ E = \int \psi^*H\psi dv \]  \hspace{1cm} (2-6)

They are listed below. The detailed expressions are in Chapt. III.
Energies are in effective Rydbergs and distances are in units of \( a_o \)
which is the radius of the first Bohr orbit for an isolated impurity
atom in a lattice without screening. The units of \( a_o \) are referred
to as effective Bohr radii. For example, phosphorous in silicon has
\( a_o \approx 20 \). The quantity \( w = \alpha R \).
\[ \int a(1)(-V_1^2)a(1)dv_1 = \alpha^2 \]  \hspace{1cm} (2-7)

\[ \int a(1)b(1)dv_1 = S = \exp(-w)(1+w+w^3/3) \]  \hspace{1cm} (2-8)

\[ \int a(1)(-V_1^2)b(1)dv_1 = -\alpha^2(K+S) \]  \hspace{1cm} (2-9)

\[ \int a^2(1)(-V_{1a})dv_1 = -2\alpha(1+\beta/2\alpha)^{-2} \]  \hspace{1cm} (2-10)

\[ \int a^2(1)(-V_{1b})dv_1 = \alpha J_s \]  \hspace{1cm} (2-11)

\[ \int a(1)b(1)(-V_{1b})dv_1 = \alpha K_s \]  \hspace{1cm} (2-12)

\[ \int a^2(1)b^2(2)(V_{12})dv_1dv_2 = \alpha J_s' \]  \hspace{1cm} (2-13)

\[ \int a(1)b(1)a(2)b(2)V_{12}dv_1dv_2 = \alpha K_s' \]  \hspace{1cm} (2-14)

All of the integrals 2-7 to 2-13 have closed analytic expressions. The last integral (Eq. 2-14) cannot be evaluated in the form of a closed analytic expression and therefore was evaluated by a process involving numerical integration (Chapt. III). Other integrals encountered in the evaluation of energy can be obtained by interchanging indices.

Thus, the ground state energy for molecules in terms of these integrals is

\[ E_{12} = (1+S^2)^{-1}[2\alpha^2(1-KS-S^2) \]

\[ \quad + \alpha(-4(1+\beta/2\alpha)^{-2} + 2J_s + J_s' + 4K_s S + K_s')] \]  \hspace{1cm} (2-15)

The term with coefficient \( \alpha^2 \) is the kinetic energy and the term with coefficient \( \alpha \) is the potential energy.
The Hamiltonian operator for a single electron bound to a pair of impurity ions separated by a distance $R$ is

$$H = -\nabla_1^2 - V_{la} - V_{lb}$$

(2-16)

The normalized wave function $\psi$ is

$$\psi = (2(1+S))^{-1}[a(l) + b(l)]$$

(2-17)

where $S = \int a(l)b(l)dv_1$ is the overlap integral as before.

The integrals needed here are as follows

$$\int a(l)b(l)dv_1 = S = \exp(-\omega)(1+\omega+\omega^3/3)$$

(2-18)

$$\int a(l)(-\nabla_1^2)a(l)dv_1 = \alpha^2$$

(2-19)

$$\int a(l)(-\nabla_1^2)b(l)dv_1 = -\alpha^2(K+S)$$

(2-20)

$$\int a(l)(-V_{la})a(l)dv_1 = -2\alpha(1+\beta/2\alpha)^{-2}$$

(2-21)

$$\int a(l)(-V_{la})b(l)dv_1 = \alpha K_s$$

(2-22)

$$\int a^2(l)(-\nabla_1^2)dv_1 = \alpha J_s$$

(2-23)

All of the integrals above have closed analytic expressions.

In terms of these integrals the binding energy for a hydrogen like molecular ion is

$$E_l = (1+S)^{-1}[\alpha^2(1-K-S) + \alpha'(J_s + 2K_s - 2(1+\beta/2\alpha)^{-2})]$$

(2-24)

The term with coefficient $\alpha^2$ is the kinetic energy and the term with coefficient $\alpha$ is the potential energy.
Equations 2-15 and 2-24 express $E_1$ and $E_{12}$ as functions of $\alpha$ with $s$ and $R$ as parameters. $E_1$ and $E_{12}$ are then minimized with respect to variational parameter $\alpha$.

2. Calculation of Fermi Energy $E_F$

The Fermi level for the intrinsic semiconductor is given by

$$E_F = \frac{E_C + E_V}{2} + \frac{kT}{2} \ln \frac{N_v}{N_c}$$

where $E_C$ is the bottom of the conduction band, $E_V$ is the top of the valence band and $N_v$, $N_c$ are defined below. $E_F$ lies very close to the center of the band gap. It shifts upwards or downwards depending on the type of impurity atoms added.

Consider the case where donor impurities of concentration $N_D (\text{cm}^{-3})$ are added to the crystal. Electrical neutrality requires that the total number of negative charges must be equal to the total number of positive charges, i.e.

$$n = N^+ + p$$  \hspace{1cm} (2-25)

where 'n' is the number of electrons in the conduction band, 'p' is the number of holes in the valence band, and $N^+$ is the number of positive charges associated with ionized donors. $N_c$ is the effective density of states in the conduction band and $N_v$ is the effective density of states in the valence band.

$$N_c = 2(2\pi m_e kT/h^2)^{3/2} N_c$$  \hspace{1cm} (2-26)

$$N_v = 2(2\pi m_h kT/h^2)^{3/2}$$  \hspace{1cm} (2-27)
$M_c$ is the number of equivalent minima in the conduction band (-6 for silicon). For an isotropic effective mass for density of states calculated in silicon values of $m_{de}$ and $m_{dh}$ are found in the literature. The numerical values obtained for $N_c$, $N_v$, $m_{de}$, and $m_{dh}$ are

$$N_c = 5.4225 \times 10^{15} T^{3/2} \text{ cm}^{-3}$$

$$N_v = 0.3719 N_c$$

$$m_{de} = 2.9801 \times 10^{-31} \text{ kg}$$

$$m_{dh} = 5.0887429 \times 10^{-31} \text{ kg}$$

Now, $N^+$, the number of ionized donors, is given by

$$N^+ = N_D \left[1 - (1 + \frac{1}{g} \exp((E_D - E_F)/kT))^3\right]$$

(2-28)

where $g$ is the ground state degeneracy of the donor impurity level ($g=2$). In the above expression all the donors have the same donor ionization energy $E_D$ valid only for very low donor concentration.

The density of electrons in the conduction band is given by

$$n = N_c 2\pi^{1/2} F_{1/2}((E_F - E_c)/kT)$$

(2-29)

where $F_{1/2}$ is the Fermi-Dirac Integral.

$$F_{1/2}(\eta_f) = \int_0^\infty \eta_f^{1/2}(1+\exp(\eta-\eta_f))^{-1} d\eta$$

(2-30)

and

$$\eta_f = (E_F - E_c)/kT$$

(2-31)
The reference level with respect to which all energies are calculated is taken as the bottom of the intrinsic conduction band, thus making \( E_c = 0 \).

\[
\psi_{1/2}(\eta_f) \text{ can be written as }
\]

\[
\psi_{1/2}(\eta_f) = \pi^{1/2} 2^{-1} \exp(\eta_f) S_M
\]

where \( S_M = 2\pi^{-1/2} \int_0^{1/2} (\exp \eta_f + \exp \eta)^{-1} \, d\eta \) \hspace{1cm} (2-32)

In the case of a nondegenerate material (Boltzmann Statistics)

\[
\psi_{1/2}(\eta_f) = (\pi^{1/2}/2)\exp(\eta_f) \text{ and consequently } B = (q^2 n/\varepsilon kT)^{1/2}.
\]

Therefore the neutrality condition \( n = N^+ \) becomes

\[
N_c \exp(\eta_f) S_M = N_D [1 + 2\exp(\eta_f - \eta_D)]^{-1} \hspace{1cm} (2-33)
\]

where \( (E_F - E_D)/kT = \eta_f - \eta_D \) \hspace{1cm} (2-33)

where \( \rho \) can be neglected at normal temperature since it is very small.

In the last case isolated singly ionized donors were considered to be present in the semiconductor. Since nearest neighbor interactions are to be taken into account, pairs of donor impurities must be considered. It is possible to have singly ionized pairs and doubly ionized pairs. The next task would then be to find the relative number density of singly and doubly ionized pairs.

From Eq. 2-28, the ratio of singly ionized donors to neutral donors is
\[ \frac{N^+}{N-N^+} = 2^{-1} \exp (n_D - n_F). \]

Let \( n_2 \): density of neutral pairs between \( R \) and \( R+dR \)

\( n_1 \): density of singly-ionized pairs between \( R \) and \( R+dR \)

\( n_0 \): density of doubly-ionized pairs between \( R \) and \( R+dR \).

\( E_1 \): binding energy of an electron to a doubly-ionized ion pair

\( E_2 \): binding energy of 2nd electron to a singly-ionized ion pair.

It will be seen that \(|E_1| > |E_2|\). Thus using the above definitions and concepts,

\[ \frac{n_1}{n_2} = g_2^{-1} \exp ((E_2 - E_F)/kT) = y_2^{-1}; \quad g_2 = 1/2 \quad (2-34) \]

\[ \frac{n_0}{n_1} = g_1^{-1} \exp ((E_1 - E_F)/kT) = y_1; \quad g_1 = 2 \quad (2-35) \]

where \( g_1 \) and \( g_2 \) are degeneracy factors. The quantities \( y_1 \) and \( y_2 \) are defined for convenience in the computer program. Now the sum of \( n_0 \), \( n_1 \) and \( n_2 \) must be the total number (cm\(^{-3}\)) of impurity pairs \( dN(R) \) between \( R \) and \( R+dR \), for small but finite \( dR \).

\[ dN(R) = n_0 + n_1 + n_2 \quad (2-36) \]

From the above equations it follows that \( n_2 \), \( n_1 \) and \( n_0 \) are

\[ n_2 = dN(R)y_2/(1 + y_1 + y_2) \quad (2-37) \]

\[ n_1 = dN(R)/(1 + y_1 + y_2) \quad (2-38) \]

\[ n_0 = dN(R)y_1/(1 + y_1 + y_2) \quad (2-39) \]
Since \( n_2 \) systems are associated with zero positive charges, \( n_1 \) systems with one positive charge and \( n_0 \) with two positive charges, the total number of positive charges \( dN^+(R) \) between \( R \) and \( R+dR \) (to give total number of ionized donors) can be obtained from

\[
dN^+(R) = 0 \cdot n_2 + 1 \cdot n_1 + 2 \cdot n_0
\]

\[
= (2dN(R))(0.5+y_1)/(1+y_1+y_2)
\]  

(2-40)

The quantities \( y_1 \) and \( y_2 \) depend on \( R \), \( E_F \), \( E_1 \) and \( E_2 \) and \( dN(R) \) depends on the probability distribution of impurities.

Therefore the total number of positive charges associated with ionized donors (singly and doubly) is

\[
N^+ = \sum_{R} dN^+(R) = \sum_{R} 2dN(R)(0.5+y_1)/(1+y_1+y_2)
\]

\[
2dN(R) = CF(R)
\]

where \( C \)=number of impurities (cm\(^{-3}\))

\( P(R) \)= probability of finding a pair with a distance between \( R \) and \( R+dR \). Therefore \( N^+ = \sum_{R} \frac{CF(R)(0.5+y_1)}{(1+y_1+y_2)} \)  

(2-41)

and \( n = N^+ \) becomes \((p<<N^+)\)

\[
N_c \exp(n_f)S_H = \sum_{R} \frac{CF(R)(0.5+y_1)}{(1+y_1+y_2)}
\]  

(2-42)

This equation can be rewritten as
\[ \exp(\eta_f) = \left(\frac{C}{N_c}\right) S^{-1} \sum_{R} F(R) \left(\frac{.5 + y_1}{1 + y_1 + y_2}\right) \quad (2-43) \]

The left-hand side obviously depends on \( \eta_f \) only. The right-hand side is a function of \( S \) and \( \eta_f \). However, \( S \) is a function of \( \eta_f \) as shown in Eq. 2-1. So the right-hand side also depends on \( \eta_f \) only. Then Eq. 2-43 can be solved by either an iterative method or by a graphical method.

3. Probability of Distribution of Impurity Pairs

The impurity concentrations of interest are of the order of \( 10^{15} \) to \( 10^{20} \) cm\(^{-3} \). In concentrations below \( 10^{20} \) cm\(^{-3} \) the number of impurities compared to the lattice sites (\( \sim 5 \times 10^{22} \) cm\(^{-3} \)) is <1:500. Also, the probability of occupation is the same for each lattice site. The probability is independent of the presence of neighbouring impurities. Poisson's statistics apply under these conditions. The probability of having \( k \) impurities in a volume \( v \), if expected number is \( Cv \) where \( C \) is the impurity concentration, is

\[ P_k(C v) = \frac{(C v)^k}{k!} e^{-C v} \]

and \( \sum_k P_k(C v) = 1 \)

The probability that there are no impurities is

\[ P_0(C v) = e^{-C v} \]

and that there is one impurity is

\[ P_1(C v) = C v e^{-C v} \]
The above is true for any volume $v$. Consider a spherical volume $v$ of radius, $R$, centered at an impurity. Then the probability of having an impurity between $R$ and $R+dR$ with an impurity at the center, and none between 0 and $R$ is

$$P(R)dR = P_0(Cv_o)P_1(Cdv)$$

where 1 represents certainty at the center, $v_o$ is the spherical volume $4\pi R^3/3$, and $dv$ is the volume of a spherical shell between $R$ and $R+dR$ given by $4\pi R^2 dR$.

Therefore

$$P(R)dR = 1 \cdot e^{-Cv_o} C \cdot 4\pi R^2 dR \cdot e^{-Cdv}$$

$$= C \cdot 4\pi R^2 dR \cdot e^{-C(v_o+dv)}$$

$$= C \cdot 4\pi R^2 dR \cdot e^{-C \cdot 4\pi R^3/3} \quad (dv \ll v_o) \quad (2-44)$$

In the following study since $R$ is in effective Bohr radii, $C$ has to be in units of inverse Bohr radii. A substitution of the form $(C R^3)^{1/3} = r$ gives

$$P(r)dr = 4\pi r^2 dre^{-4\pi r^3/3}$$

$P(R)$ is plotted for various impurity concentration $C$ in Fig. H where $C$ is in units of cm$^{-3}$, and $R$ is in units of Bohr radii.
III. CALCULATION AND RESULTS

The integrals in the expressions for $E_1$ and $E_{12}$, namely Equations 2-15 and 2-24, are evaluated here.

\[ \int a(l) (-V_1^2) a(l) dV_1 = \alpha^2 \]

\[ \int a(l) b(l) dV_1 = S = e^{-w}(1 + \nu + \frac{w^2}{3}) \]

\[ \int a(l) (-V_1^2) b(l) dV_1 = -\alpha^2(K+S) = \alpha^2 e^{-w}(1+\nu-\frac{w^2}{3}) \]

\[ \int a^2(l) (-V_{1a}^2) dV_1 = -2\alpha(1 + \frac{\beta}{2\alpha})^{-2} = -2\alpha f^2 \]

where $f = (1 + g)^{-1}$, $g = \beta/2\alpha$

\[ \int a^2(l) (-V_{1b}^2) dV_1 = \alpha J_s \text{ where} \]

\[ \alpha J_s = 2\alpha Y (e^{-2\nu} - Y (e^{-\beta R} - e^{-2\nu})/\nu) \]

and $Y = (1 - g^2)^{-2}$

Let $Y = (2\alpha - \beta)/R$

$Y_1 = (1 - e^{-Y})/Y$

$Y_2 = (1 - Y - e^{-Y})/Y^2$

$Y_3 = (1 - Y + .5Y^2 - e^{-Y})/Y^3$

$Y_4 = (1 - Y + .5Y^2 - Y^3/6 - e^{-Y})/Y^4$

Then

$Y_3 = Y \cdot Y_4 + 1/6$

$Y_2 = Y \cdot Y_3 - 1/2$
\[ Y_1 = Y \cdot Y_2 + 1 \]

By using the above definitions, the expression reduces to

\[ aJ_s = -2af e^{-BR}(2w(2fY_2 + Y_1) + f) \]

\[ \int a(1)b(1)(-v_{1b})dV_1 = aK_s \text{ where} \]

\[ aK_s = -2af^2 e^{-w(1+2w(e^{-2w}-1)/2)} \]

Let \( B_2 = (1 - BR - e^{-2w})/2 \)

Then \( aK_s = -2af^2 e^{-w(1 - 2wB_2)} \)

\[ \int a(1)b^2(2)v_{12}dV_1dV_2 = aJ_s' \text{ where} \]

\[ aJ_s' = -aw^3 \gamma(2w(2w^2+w+1)/4w^3 - e'^2/6w + e^2w(2w+1)/2w^3 \]

\[ -\gamma((a+.5\beta)R+1)e^{-(a+.5\beta)R}/wR^2(\alpha+.5\beta)^2 \]

\[ x(e^{(a-.5\beta)R} - e^{-(a-.5\beta)R})/(a-.5\beta)R \]

\[ -2fe^{-(a+.5\beta)R}/wR(a+.5\beta)[(e^{(a-.5\beta)R} - e^{-(a-.5\beta)R}) \]

\[ /2(a-.5\beta)^2R^2 - (e^{(a-.5\beta)R} + e^{-(a-.5\beta)R})/2(a-.5\beta)] \]

\[ = af^2 e^{-BR}(-w^2(4f-1)/3-w(2f^2-1)/2 + (2f^2+2f+1)/4) \]

\[ +af e^{-BR}(.5+w+2w^2/3)Y_1+2fw(1+2w)Y_2 \]

\[ +8f^2w((h+2w)Y_3+2wY_4) \]

\[ \int a(1)b(1)a(2)b(2)v_{12}dV_1dV_2 = aK_s' \]
This integral does not have a closed analytic expression. The procedure for numerically evaluating this integral is given here.

\[ \alpha_k' = \int s(\alpha_1, r_{1a}) s(\alpha_2, r_{1b}) (\exp(-\beta r_{12})/r_{12}) s(\alpha_3, r_{2a}) s(\alpha_4, r_{2b}) \]

\[ \times dv_1 dv_2 \]

\[ s(\alpha, r) = (\alpha^3/\pi)^{1/2} \exp(-ar) \]

Expand all functions in spherical harmonics about center a using

\[ (\alpha r_b)^{n-1} \exp(-\alpha r_b) = \sum_{l=0}^{\infty} (2l+1) \xi_l n(\alpha r_a, \alpha R) P_l(\cos \theta) \]

\[ \alpha_k' = \beta((\alpha_1 \alpha_2 \alpha_3 \alpha_4)^{3/2}/\pi^2) \int s(\alpha_1, r_{1a}) s(\alpha_2, r_{1b}) \]

\[ \sum_{l=0}^{\infty} (2l+1) \xi_{l,0} (\alpha r_{la}, \alpha r_{2a}) P_l(\cos \theta) \exp(-\alpha r_{2a}) \exp(-\alpha_3 r_{2a}) \]

\[ 4\beta((\alpha_1 \alpha_2 \alpha_3 \alpha_4)^{3/2}/\pi^2) \sum_{l=0}^{\infty} (2l+1) \int \exp(-\alpha_1 r_{1a}) s(\alpha_2, r_{1b}) \]

\[ \sum_{l=1}^{\infty} (2l+1) \xi_{l,1} (\alpha^3 r_{2a}, \alpha^4 R) \exp(-\alpha_3 r_{2a}) \]

\[ P_l(\cos \theta) r_{2a}^2 dr_2 dv_1 \]

\[ = 4\beta((\alpha_1 \alpha_2 \alpha_3 \alpha_4)^{3/2}/\pi) \sum_{l=0}^{\infty} (2l+1) \int \exp(-\alpha_1 r_{1a}) \]

\[ \sum_{l=1}^{\infty} (2l+1) \xi_{l,1} (\alpha^3 r_{2a}, \alpha^4 R) \exp(-\alpha_3 r_{2a}) \]

\[ P_l(\cos \theta) r_{2a}^2 dr_2 dv_1 \]
\[ \sum_{l_1=0}^{\infty} (2l_1+1) \zeta \chi_{l_1} (\alpha_2 r_{1a}, \alpha_2 R) P_{l_1} (\cos \theta_{1a}) \zeta \chi_0 (\beta r_{1a}, \beta r_{2a}) \times \exp(-\alpha_3 r_{2a}) \chi \chi_1 (\alpha_4 r_{2a}, \alpha_4 R) P_l (\cos \theta_{1a}) r_2^2 dr_2 d\omega_{1} r_1^2 dr_1 = \]

\[ 16 \beta (\alpha_1 \alpha_2 \alpha_3 \alpha_4)^{3/2} \sum_{l=0}^{\infty} (2l+1) \int \exp(-\alpha_1 r_{1a}) \zeta \chi_1 (\alpha_2 r_{1a}, \alpha_2 R) \zeta \chi_0 (\beta r_{1a}, \beta r_{2a}) \exp(-\alpha_3 r_{2a}) \chi \chi_1 (\alpha_4 r_{2a}, \alpha_4 R) r_2^2 dr_2 r_1^2 dr_1 \]

\[ \zeta \chi_0 (t_1, t_2) = i_\chi (t_\chi) k_\chi (t_\chi) \]

\[ \zeta \chi_1 (t_1, t_2) = t_\chi i_\chi (t_\chi) k_{\chi-1} (t_\chi) - t_\chi i_{\chi+1} (t_\chi) k_\chi (t_\chi) \]

where \( i_\chi (x) \) and \( k_\chi (x) \) are spherical modified Bessel functions for which the simplest are

\[ i_0 (x) = \frac{\sinh x}{x}; \quad i_{-1} (x) = \frac{\cosh x}{x} \]

\[ k_0 (x) = k_{-1} (x) = \frac{e^{-x}}{x} \]

and the recursion relations are

\[ i_{\chi-1} (x) = i_{\chi+1} (x) + ((2\chi+1)/x) i_\chi (x) \]

\[ k_{\chi+1} (x) = k_{\chi-1} (x) + ((2\chi+1)/x) k_\chi (x) \]

In terms of these functions, the scaled spherical Bessel Functions are defined as

\[ i_\chi^{s} (x) = ((2\chi+1)!!/x^\chi) \exp(-x) i_\chi (x) \]
\[ k^s_\ell(x) = \left(\frac{x^{\ell+1}}{(2\ell+1)!!}\right) \exp(x) k^s_\ell(x) \]

where \((2\ell+1)!! = 1 \cdot 3 \cdot \ldots \cdot (2\ell+1)\) is the "odd number factorial".

In terms of these scaled functions

\[ (2\ell+1)B^s_{\ell,0}(\beta_{r_1},\beta_{r_2}) = \left(\frac{r_<}{r_>}\right)^{\ell+1} i^s_\ell(\beta_{r_<}) k^s_\ell(\beta_{r_>}) \exp(-\beta(r_->r_<)) \]

\[ \tau^s_{\ell,1}(\alpha_4 r_{2a},\alpha_4 R) = \alpha_4 \exp(-\alpha_4 (r_> - r_<)) \times \]

\[ \left(\left(\frac{1}{(2\ell+1)(2\ell+2)}\right) r_<^{\ell+2} r_>^{\ell+1} i^s_{\ell+1}(\alpha_4 r_<) k^s_\ell(\alpha_4 r_<) k^s_\ell(\alpha_4 r_>\right) \]

In order to avoid negative indices, use is made of \( k_0 = k_{-1} \) so that for the \( \ell = 0 \) case

\[ \tau^s_{0,1}(\alpha_4 r_{2a},\alpha_4 R) = (i^s_0(\alpha_4 r_<) \alpha_4 r_> - i^s_1(\alpha_4 r_<) \alpha_4 r_<^2/3r_> \times \]

\[ k_0^s(\alpha_4 r_<) \exp(-\alpha_4 (r_> - r_<)) \]

\( K^s \) is a function of \( \alpha, \beta, \) and \( R \). However, with the substitution \( g = \beta/2a \) and \( w = \alpha R \), \( K^s \) is reduced to a function of \( g \) and \( w \). For \( w \) from 0 to 8 in steps of 0.2, and \( g \) from 0 to 2.4 in steps of 0.1, \( K^s \) was calculated with a computer program (V. Kapadia). With these calculated values, it is possible to find a simple function to fit them. Because for \( R = 0 \), i.e. \( w = 0 \), \( K^s \) can be computed exactly.
as \( K'_s(g,0) = 0.25 [(1 + g)^{-2} + 2(1+g)^{-3} + 2(1+g)^{-4}] \), a function of the form \( K'_s(g,0) \exp(-2w) \{1 + A_{1g}w + A_{2g}w^2 + A_{3g}w^3 + A_{4g}w^4\} \) is chosen to fit the calculated values of \( K'_s \). \( A_{1g}, A_{2g}, A_{3g}, \) and \( A_{4g} \) are determined for \( g \) from 0 to 2.4 in steps of 0.1 by using the least square-error fit method. The resulting function is accurate to four decimal places. Values of \( A_{1g}, A_{2g}, A_{3g}, \) and \( A_{4g} \) are shown in STM\( (K,w,ww) \) function subroutine of Appendix B. STM is \( A_{1g} + A_{2g}w + A_{3g}w^2 + A_{4g}w^3 \), \( K \) is the integer part of \( 10g \), and \( ww \) is \( w^2 \), it is easy to see that, e.g., \( A_{1g} = 2.00243 \) for \( 0 < g < 0.1 \), and \( A_{1g} = 2.00196 \) for \( 0.1 < g < 0.2 \). With this functional form of \( K'_s \) and all the other integrals previously shown, \( E_1 \) and \( E_{12} \) are evaluated by EE\( (I,A,R,B) \) function subroutine in Appendix B. \( E_1 \) is EE\( (1,A,R,B) \). \( E_{12} \) is EE\( (2,A,R,B) \), \( A \) is \( \alpha \), and \( B \) is \( B \). \( E_1 \) and \( E_{12} \) are plotted in Fig. E and Fig. F as a function of variational parameter \( \alpha \) for various values of \( B \) and \( R \) by calling subroutine EAA. The curves are seen to be smooth, and each one has a single minimum. This suggests that the chosen trial function as shown in Eq. 2-5 is a reasonable one. Next step is to minimize \( E_1 \) and \( E_{12} \) with respect to \( \alpha \). For this purpose, a numerical technique assuming the curve is a parabola near its minimum is used to find the minimum value. This is done by subroutine AME. The results are shown in Fig. G where minimized \( E_1, E_{12} \) (actually \( E_2 = E_{12} - E_1 \)), and the corresponding \( \alpha \) values (denoted as \( \alpha_1 \) and \( \alpha_{12} \)) are plotted as a function of \( R \) with \( B \) as a parameter by calling subroutine EAR.

Fermi energy \( E_f \) is determined by solving Eq. 2-43. In order to solve Eq. 2-43 by a numerical approximation method, \( \delta \) needs to be
expressed in terms of \( \eta_f \). From Eq. 2-1, 2-29, and 2-32, \( \beta \) is

\[
\beta = \left( \frac{q^2}{(\varepsilon k T)} \right)^{1/2} \frac{d}{d\eta_f} \left( \exp(\eta_f) S_N \right)^{1/2}
\]

\[
= \left( \frac{q^2}{(\varepsilon k T)} \right)^{1/2} N_c S_N^{1/2} \tag{3.1}
\]

where \( S_N = 2 \pi^{-1/2} \exp(\eta_f) \int_0^{\eta_f} \exp(\eta) \left( \exp(\eta_f) + \exp(\eta) \right)^{-2} d\eta \)

\( y_1 \) and \( y_2 \) in the right-hand side of Eq. 2-43 are functions of \( E_1 \) and \( E_2 \) which in turn depends on \( \beta \). By using Eq. 3-1, \( y_1 \) and \( y_2 \) can be evaluated as functions of \( \eta_f \). Therefore, other than some physical constants, the right-hand side of Eq. 2-43 can be calculated as a function of \( \eta_f \). As an example, the physical constants are chosen for silicon doped with phosphorus atoms, then logarithm of the right-hand side of Eq. 2-43 is calculated by YF function subroutine. Logarithm of both sides of Eq. 2-43 are shown in Fig. 1 as a function of \( \eta_f \) for various values of the impurity concentration \( C \) and temperature \( T \) by calling FxF subroutine. The diagonal straight line is obviously the logarithm of left-hand side, and the curve that resembles a third-order polynomial is the logarithm of right-hand side. The intercept of the two gives the solution to Eq. 2-43. The intercept, or intercepts - if there are more than one, is determined by numerical techniques shown in subroutines ROOT and FNRT.

Thus Fermi energy \( E_F \) is determined as a function of \( C \) and \( T \). Once this is done, the screening factor \( \beta \) can be determined with
Eq. 3-1, and the free carrier concentration \( n \) can be determined with Eq. 2-29, \( E_F \), \( B \), and \( n \) are plotted as a function of \( T \) for various values of \( C \) in Fig. B, C, and D by calling subroutine \( \text{EFBN} \). Once \( B \) is determined as a function of \( C \) and \( T \), \( E_1 \) and \( E_2 \) can be calculated as a function of \( R \), \( C \), and \( T \). \( E_1 \), \( E_2 \), and probability of distribution \( P \) are plotted in Fig. A.1.A to A.64.A as a function of \( R \) for various values of \( C \) and \( T \) by calling subroutine \( \text{PER} \).

The densities of states \( S_1(E) \) and \( S_2(E) \) are calculated by transforming \( P(R) \) and \( E_1(R) \) into \( S_1(E) \), and \( P(R) \) and \( E_2(R) \) into \( S_2(E) \). \( S_1(E) \) is the density of those donor pairs for which the energy needed to ionize a single localized electron equals \( E \). \( S_2(E) \) is the density of those donor pairs for which the energy needed to ionize one of two localized electrons equals \( E \). It is interesting to calculate the density of filled states, \( F_1(E) \) and \( F_2(E) \). This is because \( F_1(E) \) and \( F_2(E) \) are not simply \( S_1(E) \) and \( S_2(E) \) multiplied by a factor corresponding to Fermi statistics. Each donor pair could have two, one, or zero electrons. \( F_2(E) \) is the portion of \( S_2(E) \) which have two localized electrons. \( F_1(E) \) is the portion of \( S_1(E) \) which have either one or two localized electrons. \( S_1 \), \( S_2 \), \( F_1 \) and \( F_2 \) are calculated with procedures in subroutine \( \text{SFE} \). They are plotted in Fig. A.1.B to A.64.B as a function of \( E \) for various values of \( C \) and \( T \) by calling subroutine \( \text{SFE} \). \( E = 0 \) corresponds to the conduction band edge for \( C \to 0 \).

The computer program is written in Fortran and shown in Appendix B. The main program explains how to call each subroutine that plots calculated results.
IV. SUMMARY AND DISCUSSION

Fig. K and F show binding energies $E_1$ and $E_{12}$ as a function of variational parameter $\alpha$. Each curve closely resembles a parabola. It is fast and accurate to determine the minimum values of $E_1$ and $E_{12}$ by assuming that $E_1(\alpha)$ and $E_{12}(\alpha)$ are parabolas near their minima. The minimized $E_1$ and $E_2(=E_{12}-E_1)$, together with the corresponding values of $\alpha$, are shown in Fig. G. As expected, the absolute values of $E_1$ and $E_2$ decrease as either $B$ or $R$ increases. This is because larger $B$ means stronger screening, and larger $R$ means donors are farther apart, both of which reduce binding energies for localized electrons. The same can be said of values of $\alpha$ which minimize $E_1$ and $E_2$, because both stronger screening and larger inter-donor distance have the effect of delocalizing wave functions of localized electrons, i.e., reducing $\alpha$. Fig. G shows that $E_1$, $E_2$, and the corresponding $\alpha_1$ and $\alpha_{12}$ follow this rule. It is also interesting to compare the calculated values with known values for the special cases where $B = 0$, and $R = 0$ or $R \to \infty$. For $B = 0$, Fig. G shows that $\alpha_1 = 2$ at $R = 0$, and $\alpha_1 \to 1$ as $R \to \infty$, both of these match the expected values. It also shows that, for $B = 0$, $\alpha_{12} \sim 1.7$ at $R = 0$, and $\alpha_{12} \to 1$ as $R \to \infty$. The former matches the calculation done by Merzbacher, and the latter is obviously true. The same can be said of the trivial fact that $E_1 = -4$ for $R = 0$, and $E_1 \to -1$ as $R \to \infty$. It can also be
seen that $E_2 \sim -1.7$ for $R = 0$, and $E_2 \to -1$ as $R \to \infty$. The former is reasonably close to the experimental value of $-1.8$ (Merzbacher), and the latter is trivial. It is also expected that $\alpha_1, \alpha_{12}, E_1$, and $E_2 \to 0$ as $B$ becomes large. This is true of Fig. 6 where $\alpha_1, \alpha_{12}, E_1$, and $E_2 \sim 0$ for $B \geq 2$.

Fig. I shows how Eq. 2-43 is solved by a graphical or numerical approximation method. The intercept of the diagonal and the curve gives the Fermi energy that satisfies Eq. 2-43, as explained in Chapt. III. One intriguing result is that the diagonal intercepts the curve three times for impurity concentration $C \geq 10^{18}$ cm$^{-3}$ and temperature $T \leq 40$ K. This means that there are three solutions to Eq. 2-43 under these conditions. Discarding the middle value as unstable, this leaves two stable Fermi energies. Once Fermi energy $E_F$ is determined, screening factor $B$, free electron concentration $n$, density of states $S$ and filled states $F$, and ground state energies $E_1$ and $E_2$ can all be calculated as functions of $C$ and $T$. The results are shown in Fig. A to Fig. D.

In Fig. A.1.A to A.6.A, it is seen that the percentage of donor pairs whose localized electron binding energies are appreciably different from that of isolated donors is rather low for $C \leq 10^{17}$ cm$^{-3}$. To be more specific, for $C = 10^{17}$ cm$^{-3}$, the most probable inter-atom distance for donor pairs is about 6 Bohr radii, while donors can roughly be considered as being isolated for inter-donor distance larger than 4 Bohr radii. On the other hand, when $C$ is increased to $10^{19}$ cm$^{-3}$, it can be seen that virtually none of
the donor pairs can be treated as isolated donors. This indicates that interactions beyond pair level are not important for $C$ up to $10^{18}$ cm$^{-3}$ where a noticeable portion of donor pairs can actually be treated as isolated donors. Furthermore, if it is assumed that electrons have pairing habits, the pair model is presumably good for considerably higher $C$.

In Fig. A.1.B to A.64.B, the energy spectrum is shown. As expected, the impurity band broadens as $C$ increases (Bonch-Bruyevich\textsuperscript{1}, W. Y. Ching\textsuperscript{18}) up to $10^{18}$ cm$^{-3}$. It is also seen that ionization is quite negligible for $T \leq 40$ K which is sufficiently low for the n-silicon to be used as an infrared detector. For any higher $C$, the screening is sufficiently strong that impurity band shrinks and merges with conduction band. This is in agreement with previous works (Bonch-Breyevich\textsuperscript{7,8}).

Fig. B, C, and D show Fermi energy $E_F$, screening factor $\beta$, and free electron concentration $n$ as functions of $T$ for various values of $C$. It is noticed that $E_F$ actually goes into conduction band for $C \geq 10^{18.5}$ cm$^{-3}$ at low temperatures. This would give rise to Burstein-Moss\textsuperscript{15,16} effect as mentioned in Chapt. I.

For $C \geq 10^{18}$ cm$^{-3}$ and $T \leq 40$ K, the semiconductor could be in another stable state. This is seen in Fig. A, B, C, and D at the corresponding $C$ and $T$. This state has a lower Fermi energy, lower screening factor, lower free electron concentration, and an impurity band that is broader and farther away from conduction band. All these are consistent with one another. If the initial temperature is $\sim 0$ K, then nearly all the electrons are localized which, in turn,
results in little screening. Low screening leads to a broad impurity band that is separated from conduction band. This, in turn, leads to a low Fermi energy. The fact that lower Fermi energy means more localized electrons completes the self-consistent cycle. With increasing temperature, Fermi energy $E_F$ and screening factor $S$ increase in a roughly exponential way, slowly at first, but gradually getting faster until at $T \sim 40$ K where they rise sharply to the values which they would have had if the initial temperature were high instead of 0 K. Obviously, with a high initial temperature, the semiconductor would retain sufficient free electrons to remain in the state where the screening is high when temperature is lowered. Presumably, the semiconductor would remain in this state until $T \sim 0$ K where screening becomes negligibly low.

What this implies is that the state of the semiconductor depends on its temperature history at the concentration and temperature ranges just mentioned. Some experimental evidences (W. P. Rahilly$^{39}$, D. P. Jayapandian$^{40}$, C. G. Noll$^{41}$, S. C. Yerian$^{42}$) support the foregoing theory. In an experiment conducted in Dr. L. C. Brown's lab, it was found that the signal strength of electron spin resonance at 30 K of a phosphorus doped silicon sample depended on its temperature history prior to the time when data was taken. This indicates that the silicon could be in one state or the other depending on its previous temperature. In another experiment, the nuclear spin-lattice relaxation time $T_1$ was measured. As it turned out, $T_1$ had different values at $T < 40$ K again depending on temperature history. This indicates that the silicon could be in different states, so that
the interaction between silicon 29 nuclei and surrounding electrons is uncertain, in one case with conduction electrons and in the other with localized electrons.

The range of donor concentration where donor-pair effects dominate was studied by G. A. Thomas. The randomness of donor positions naturally leads to the conclusion that as the donor concentration is increased, the first effect on the isolated donor is due to its nearest neighbor. That means that the major effects are due to the pairs of donors which are closer than average (Golka, Bhatt, Thomas). The most probable nearest-neighbor distance is $r_{NN} \approx 0.54 r_c$ where $r_c \equiv C^{-1/3}$ is the nearest-neighbor distance on a simple cubic lattice at the same density. The $1s$ wave function is of the form $e^{-r/a}$, where $a$ is the Bohr radius. For $n$-silicon, $a \approx 20 \, \text{Å}$. The effect on the $1s$ state is studied by comparing the overlap of the nearest neighbor with the overlap of the six nearest neighbors in a simple cubic lattice. The ratio $R^*$ is defined as

$$R^* = 6 \exp(-r_c/a)/\exp(-r_{NN}/a)$$

For $C = 10^{18} \, \text{cm}^{-3}$, $R^* \sim 0.6$. For $R^*$ less than 1, pair effects make major contributions. Therefore pair effects dominate for $C$ up to $10^{18} \, \text{cm}^{-3}$. Using tight binding method, W. Y. Ching obtained similar results. He showed that electron wave-functions are essentially confined within the nearest neighbors for $r_c/a \geq 5$, or $C \leq 10^{18} \, \text{cm}^{-3}$ for $a = 20 \, \text{Å}$. This agrees with previous discussions. As impurity concentration is increased, the potential range is reduced because screening factor $\beta$ increases. This implies that
screening effect enhances interactions within pairs relative to that within clusters bigger than pairs. In fact, the reduction of binding energies resulting from the increase in screening means that some donor pairs can be regarded as being isolated donors. This makes the interactions beyond pair level relatively unimportant. Furthermore, considering the fact that electrons in different spin states could be in the same orbital state, it might be assumed that electrons have the habit of forming pairs. This would make the pair model plausible for even higher impurity concentrations.

In the absence of screening, the impurity band would be rather broad. J. R. Lowney measured the band gap narrowing in the depletion layer of silicon diodes. Naturally, there is no screening effect in the depletion layer. He found that the band gap narrowing is up to 0.5 V for \( C = 1.4 \times 10^{19} \text{ cm}^{-3} \). This supports the result in the present work where it is shown that the impurity band is broad at \( C = 10^{19} \text{ cm}^{-3} \) in the state where there is little screening. On the other hand, in the presence of screening, the gap narrowing is about 0.1 V for the same concentration (Neugroschel).

Strictly speaking, the linearized classical screening theory is valid only for high impurity concentrations (Shklovskii). The quantum mechanical version is of longer range (W. A. Harrison). Furthermore, more sophisticated trial functions could be used for calculations of ground state energies. For example, C. L. Pekeris calculated ionization potential of helium \((R = 0)\) accurate to \(10^{-6}\) using trial functions with more than one variational parameter.
However, there is little justification to use either quantum screening theory or more complicated trial functions to calculate ground state energies.

The importance of screening in the determination of the energy spectrum is rather evident, both from the present work and previous works (Bonch-Bruevich, Mahan, Berggren). J. R. Lowney's experiment showed that band structure is drastically changed when screening is absent as compared with the cases when it is present. D. K. Ferry provided further evidence by studying intrinsic semiconductors under intense laser irradiation. He found that the band structure is strongly controlled by the screening effect resulting from the optically generated electrons and holes. As for the potentials of ionized donors, it has been shown that they can be limited to pairs in a good approximation. By combining pair interactions with screening effect, the major interactions in a semiconductor are taken into account for a wide range of impurity concentration.

In the present work, the density of states for localized impurity electrons was calculated and plotted relative to the unperturbed intrinsic conduction band edge which was chosen as the zero energy reference. The actual conduction band edge moves toward the valence band as impurity concentration is increased. Similarly, the actual valence band edge moves toward the conduction band. This effect is known as band gap narrowing. The band gap narrows because of conduction band electron-electron interactions and also by scattering interactions with impurity atoms. The band gap is further narrowed by the screening and neighbor-interactions considered in
this study. The activation energy of an electron-hole pair is reduced because of screening and the actual conduction band edge is lower than that in intrinsic material because of increasing potential well overlap with increasing impurity concentration.

SUMMARY
1. Ground state energies of localized electrons in a screened donor pair were calculated over a wide range of donor concentrations and temperatures. This was done by a variational method.
2. The Fermi energy and density of states were calculated from the above energies and the probability distribution of the pair separations.
3. The present model applies at low, moderate and high doping levels and is in substantial agreement with experimental results reported in the literature.
4. The impurity band broadens as impurity concentration is increased and shows an asymmetric distribution with a 'tail' extending well into the band gap, due primarily to neighbor interactions.
5. The impurity band approaches and merges with the conduction band as concentration increases, due primarily to screening. This agrees with known experimental results (Pearson, Fritzsch).
6. The most interesting result of present work is that for \( C \geq 10^{18} \text{ cm}^{-3} \) and \( T \leq 40 \text{ K} \), the semiconductor has two stable states. In one state the impurity band is broad and separated from the conduction band, in the other state the impurity band merges with the
conduction band. Obviously, screening is weak in one state and strong in the other. Earlier experimental effects (Rahilly\textsuperscript{39}, Jayapandian\textsuperscript{40}, Noll\textsuperscript{41}, Yerian\textsuperscript{42}) are consistent with this result.

7. Band gap narrowing effects are indicated by the calculation and are shown to depend on both the screened potential and the overlap of potential wells.

8. At low temperature, the behavior of the Fermi energy and the impurity band provide insight into the performance of a diode as an infrared detector.

Note: PLT$TL$, PLT$PT$, etc. in the computer program are subroutines written by high-energy physics group of Ohio State University for plotting graphs.
APPENDIX A

CALCULATED RESULTS IN GRAPHICAL FORM
$P, E_1, E_2$ VS. $R$

FIG. A.1.A  PROBABILITY $P$ AND GROUND STATE ENERGY $E$ VS. IMPURITY DISTANCE $R$. $B$ IS SCREEN FACTOR (IN $1/BR$), $EF$ IS FERMI ENERGY (IN $POB$).
FIG. A.2.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RCB).
FIG. A.4.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RD3).
$P, E_1, E_2$ vs. $R$

FIG. A.5.A PROBABILITY $P$ AND GROUND STATE ENERGY $E$ VS. IMPURITY DISTANCE $R$. $B$ IS SCREEN FACTOR (IN $1/BR$), $EF$ IS FERMI ENERGY (IN $RDB$).
FIG. A.7.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BA), EF IS FERMI ENERGY (IN RDB).
Fig. A.8.a  Probability $P$ and ground state energy $E$ vs. impurity distance $R$. $B$ is screen factor (in $1/BR$), $EF$ is Fermi energy (in $RDB$).
P, E1, E2 VS. R

FIG. A.9.A  PROBABILITY P AND GROUND STATE ENERGY E VS.
IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/Å). EF IS
FERMI ENERGY (IN RDB).
P, E₁, E₂ VS. R

E₁, E₂ (RDB), P (ARB. UNIT)

R (BR)

LOG C=16.5
T=20
B=0.00
EF=-0.55

FIG. A.10.A PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB).
P, E1, E2 VS. R

LOG C = 16.5
T = 40
B = 0.03
EF = -0.63

FIG. A.11.A  PROBABILITY P AND GROUND STATE ENERGY E VS.
IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS
FERMI ENERGY (IN ROB).
$P, E_1, E_2$ VS. $R$

Fig. A.14.A  Probability P and ground state energy E vs. impurity distance R. B is screen factor (in 1/BR), EF is Fermi energy (in ROB).
FIG. A.15.A PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB).
$P, E_1, E_2$ VS. $R$

**FIG. A.18.A**  PROBABILITY $P$ AND GROUND STATE ENERGY $E$ VS. IMPURITY DISTANCE $R$. $B$ IS SCREEN FACTOR (IN 1/BR), $EF$ IS FERMI ENERGY (IN RDB).
FIG. A.20A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR). EF IS FERMI ENERGY (IN RDB).
$P, E_1, E_2$ VS. $R$

![Graph showing $P, E_1, E_2$ vs. $R$]

FIG. A.22.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB).
Probability $P$ and ground state energy $E$ vs. impurity distance $R$. $B$ is screen factor (in $1/BR$), $EF$ is Fermi energy (in $RDB$).

- $LOG C = 17.0$
- $T = 300$
- $B = 0.15$
- $EF = -3.32$
FIG. A.24A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB).
P, E1, E2 vs. R

Fig. A.25A  Probability P and ground state energy E vs. impurity distance R. B is screen factor (in 1/BR), EF is Fermi energy (in RDB).
P, E1, E2 VS. R

Fig. A.26. A probability P and ground state energy E vs. impurity distance R. B is screen factor (in 1/BR), EF is Fermi energy (in RDB).
FIG. A.27.A  PROBABILITY P AND GROUND STATE ENERGY E VS.
IMPURITY DISTANCE R.  B IS SCREEN FACTOR (IN 1/BR), EF IS
FERMI ENERGY (IN RDB).

\[
\text{LOG } C = 17.5 \\
T = 40 \\
B = 0.08 \\
EF = -0.47
\]
$P, E_1, E_2$ vs. $R$

**Figure A.28.A**  Probability $P$ and ground state energy $E$ vs. impurity distance $R$. $B$ is screen factor (in $1/BR$), $EF$ is Fermi energy (in RDB).
**P, E1, E2 VS. R**

FIG. A.29.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB).
FIG. A.30.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RCB).
P, E1, E2 VS. R

FIG. A.31.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RD3).
FIG. A.33A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB).
FIG. A.34.A PROBABILITY $P$ AND GROUND STATE ENERGY $E$ VS. IMPURITY DISTANCE $R$. $B$ IS SCREEN FACTOR (IN $1/BR$), $EF$ IS FERMI ENERGY (IN ARS).
P, E1, E2 vs. R

Fig. A.36.a  Probability P and ground state energy E vs. impurity distance R. B is screen factor (in 1/BR), EF is Fermi energy (in RdB).
$P, E_1, E_2$ vs. $R$

**FIG. A.37.A** PROBABILITY $P$ AND GROUND STATE ENERGY $E$ VS. IMPURITY DISTANCE $R$. $B$ IS SCREEN FACTOR (IN $1/BR$), $EF$ IS FERMI ENERGY (IN RDB).
FIG. A.38.A  PROBABILITY P AND GROUND STATE ENERGY E VS.
IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR). EF IS
FERMI ENERGY (IN RDS).

LOG C=18.0
T=200
B=0.53
EF=-1.15
$P, E_1, E_2$ vs. $R$

FIG. A.40.A  PROBABILITY $P$ AND GROUND STATE ENERGY $E$ VS. IMPURITY DISTANCE $R$. $B$ IS SCREEN FACTOR (IN $1/BR$), $EF$ IS FERMI ENERGY (IN ROB).
Figure A.41A shows the probability P and ground state energy E vs. impurity distance R. B is the screening factor (in 1/BR), EF is the Fermi energy (in RDB).
FIG. A.42.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR). EF IS FERMI ENERGY (IN RDB).
$P, E_1, E_2$ VS. $R$

- $P, E_1, E_2$ (arb. unit)
- $R$ (arb. unit)

Log $C = 18.5$
$T = 40$
$B = 1.31$
$E_F = 0.02$

FIG. R.43A  PROBABILITY $P$ AND GROUND STATE ENERGY $E$ VS. IMPURITY DISTANCE $R$. $B$ IS SCREEN FACTOR (IN 1/BR), $E_F$ IS FERMI ENERGY (IN RDB).
FIG. A.44.A  PROBABILITY $P$ AND GROUND STATE ENERGY $E$ VS. IMPURITY DISTANCE $R$. $B$ IS SCREEN FACTOR (IN $1/BR$), $EF$ IS FERMI ENERGY (IN $RDB$).
P, E1, E2 VS. R

FIG. A.45.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB).
$P, E_1, E_2$ vs. $R$

**Figure A.46A**: Probability $P$ and ground state energy $E$ vs. impurity distance $R$. $B$ is screen factor (in $1/R_B$). $E_F$ is Fermi energy (in RDB).
P, E1, E2 vs. R

FIG. 47. A probability P and ground state energy E vs. impurity distance R. B is screen factor (in 1/BR), EF is Fermi energy (in RDB).
FIG. A.48.A PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB)
P, E1, E2 VS. R

P, E₁, E₂ VS. R

FIG. A.50.A  PROBABILITY P AND GROUND STATE ENERGY E VS.
IMPURITY DISTANCE R.  B IS SCREEN FACTOR (IN 1/BR), EF IS
FERMI ENERGY (IN RDB).
P, E1, E2 VS. R

FIG. A.51.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R.  B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB).
P, E1, E2 VS. R

LOG C = 19.0
T = 60
B = 1.65
EF = 0.09

FIG. A.52.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR). EF IS FERMII ENERGY (IN RDB).
E1, E2 (RDB), P (ARB. UNIT)

\[
\begin{align*}
&-4.000 \quad -3.000 \quad -2.000 \quad -1.000 \quad 0.000 \quad 1.000 \\
&0.000 \quad 2.000 \quad 4.000 \quad 6.000 \quad 8.000
\end{align*}
\]

P, E1, E2 VS. R

\[
\begin{align*}
\text{LOG C} &= 19.0 \\
T &= 200 \\
B &= 1.41 \\
EF &= -0.29
\end{align*}
\]

FIG. 54.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR). EF IS FERMIO ENERGY (IN RDB).
FIG. A.56.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB).
Fig. A.57a  Probability P and ground state energy E vs. impurity distance R. B is screen factor (in 1/BR). EF is Fermi energy (in ROB).
**FIG. A.58.A** PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR). EF IS FERMI ENERGY (IN RDB).
P, E₁, E₂ VS. R

FIG. A.59.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB).
FIG. A.60.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR). EF IS FERMI ENERGY (IN RDB).
$P, E_1, E_2$ vs. $R$

![Diagram showing $P, E_1, E_2$ vs. $R$.]

**Fig. A.61.A** Probability $P$ and ground state energy $E$ vs. impurity distance $R$. $B$ is screen factor (in $1/\text{BR}$), $EF$ is Fermi energy (in RDB).
P,E1,E2 VS. R

FIG. A.62.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR), EF IS FERMI ENERGY (IN RDB).
$P, E_1, E_2$ vs. $R$

$E_1, E_2$ (RDB), $P$ (ARB. UNIT)

$T = 300$

$B = 1.86$

$E_F = 0.14$

LOG $C = 19.5$

FIG. A.63.A  PROBABILITY $P$ AND GROUND STATE ENERGY $E$ VS. IMPURITY DISTANCE $R$. $B$ IS SCREEN FACTOR (IN $1/BR$), $E_F$ IS FERMI ENERGY (IN RDB).
FIG. A.64.A  PROBABILITY P AND GROUND STATE ENERGY E VS. IMPURITY DISTANCE R. B IS SCREEN FACTOR (IN 1/BR). EF IS FERMI ENERGY (IN RDB).
$S_1, S_2, F_1, F_2 \text{ VS. } E$

LOG $C=16.0$

$T=10$

$EF=-0.53$

**FIG. A.1.B** DENSITY OF STATES $S_1, S_2$ AND FILLED STATES $F_1, F_2$ VS. ENERGY $E$. $EF$ IS FERMI ENERGY.
FIG. A.2.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY $E$. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

FIG. A.3.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.4.B  DENSITY OF STATES $S_1, S_2$ AND FILLED STATES $F_1, F_2$ VS. ENERGY $E$. $EF$ IS FERMI ENERGY.
FIG. A.5.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

FIG. A.6.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
Fig. A.7.8  Density of states $S_1, S_2$ and filled states $F_1, F_2$ vs. energy $E$. $E_F$ is Fermi energy.
S1, S2, F1, F2 VS. E

LOG C = 16.0
T = 400
EF = -6.56

FIG. A.8.8 DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C = 16.5
T = 10
EF = -0.51

FIG. A.9.6  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
\textbf{S1, S2, F1, F2 VS. E}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figA10b.png}
\caption{Density of states S1, S2 and filled states F1, F2 vs. energy $E$. $E_F$ is Fermi energy.}
\end{figure}

\texttt{LOG C=16.5}
\texttt{T=20}
\texttt{EF=-0.55}
S1, S2, F1, F2 VS. E

Log C = 16.5
T = 40
EF = -0.63

Fig. A.11.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
$S_1, S_2, F_1, F_2$ VS. $E$

Fig. A.12.8 Density of states $S_1, S_2$ and filled states $F_1, F_2$ vs. energy $E$. $E_F$ is Fermi energy.
FIG. A.13.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C = 16.5
T = 200
EF = -2.43

FIG. A.14.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
$S_1, S_2, F_1, F_2$ vs. $E$

Log $C = 16.5$

$T = 300$

$E_F = -3.99$

FIG. A.15.B DENSITY OF STATES $S_1, S_2$ AND FILLED STATES $F_1, F_2$ vs. ENERGY $E$. $E_F$ IS FERMI ENERGY.
FIG. A.16.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.17.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.18.B  DENSITY OF STATES S1,S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
SI, S2, F1, F2 VS. E

LOG C = 17.0
T = 40
EF = -0.55

FIG. A.19.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.20.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.21.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C=17.0
T=200
EF=-1.99

FIG. A.22.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.23.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

FIG. A.24.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C = 17.5
T = 10
E_F = -0.47

Fig. A.25.8  Density of states S1, S2 and filled states F1, F2 vs. energy E. E_F is Fermi energy.
S1, S2, F1, F2 VS. E

$log C = 17.5$

$T = 20$

$EF = -0.49$

FIG. A.26.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.27.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.28.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.29.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.30.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C = 17.5
T = 300
EF = -2.67

FIG. A.31.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

FIG. A.32.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

FIG. A.33.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A34.B  DENSITY OF STATES $S_1, S_2$ AND FILLED STATES $F_1$, $F_2$ VS. ENERGY $E$. $E_F$ IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C = 18.0
T = 40
EF = -0.20

FIG. A.35.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.36.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C = 18.0
T = 100
EF = -0.42

Fig. A.37.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C = 18.0
T = 200
EF = -1.15

FIG. A.38.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C = 18.0
T = 300
EF = -2.02

FIG. A.39.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
\[ S_1, S_2, F_1, F_2 \text{ VS. } E \]

\[ \log C = 18.0 \]
\[ T = 400 \]
\[ E_F = -3.00 \]

**FIG. A.40.B** DENSITY OF STATES $S_1, S_2$ AND FILLED STATES $F_1, F_2$ VS. ENERGY $E$. $E_F$ IS FERMI ENERGY.
S1, S2, F1, F2 vs. E

FIG. A.41.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
$S_1, S_2, F_1, F_2$ VS. $E$

LOG $C = 18.5$

$T = 20$

$E_F = 0.05 - 0.46$

FIG. A.42.B  DENSITY OF STATES $S_1, S_2$ AND FILLED STATES $F_1, F_2$ VS. ENERGY $E$. $E_F$ IS FERMI ENERGY.
$S_1, S_2, F_1, F_2$ vs. $E$

FIG. R.43.B DENSITY OF STATES $S_1, S_2$ AND FILLED STATES $F_1, F_2$ vs. ENERGY $E$. $E_F$ IS FERMI ENERGY.
FIG. A.44.B  DENSITY OF STATES S1,S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

$\text{LOG C}=18.5$
$T=100$
$\text{EF}=-0.19$

FIG. A.45.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
F1, F2 VS. E

LOG C = 18.5
T = 200
EF = -0.71

Fig. A46.B  Density of states S1, S2 and filled states F1, F2 vs. energy E. EF is Fermi energy.
LOG $C = 18.5$
$T = 300$
$EF = -1.37$

**FIG. A.47.B** DENSITY OF STATES $S_1, S_2$ AND FILLED STATES $F_1, F_2$ VS. ENERGY $E$. $EF$ IS FERMI ENERGY.
FIG. A.48.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
$S_1, S_2, F_1, F_2$ VS. $E$

LOG $C = 19.0$
$T = 10$
$E_F = 0.07$ - $0.48$

FIG. A.49.B  DENSITY OF STATES $S_1, S_2$ AND FILLED STATES $F_1, F_2$ VS. ENERGY $E$. $E_F$ IS FERMI ENERGY.
FIG. A.50.B  DENSITY OF STATES $S_1, S_2$ AND FILLED STATES $F_1$, $F_2$ VS. ENERGY $E$. EF IS FERMII ENERGY.
LOG $C = 19.0$
$T = 40$
$EF = 0.09$

**FIG. A.51.B**  DENSITY OF STATES $S1, S2$ AND FILLED STATES $F1, F2$ VS. ENERGY $E$. $EF$ IS FERMI ENERGY.
FIG. A.52.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.53.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.54.B  DENSITY OF STATES S1,S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.55.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C=19.0
T=400
EF=-1.29

FIG. A.56.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.57.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

FIG. A.58.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C = 19.5
T = 40
EF = 0.15 - 0.32

FIG. A.59.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C = 19.5
T = 60
EF = 0.18

FIG. A.60.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

![Graph showing density of states S1, S2, and filled states F1, F2 vs. energy E. EF is Fermi energy.](image_url)

FIG. A.61.B DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.62.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
S1, S2, F1, F2 VS. E

LOG C = 19.5
T = 300
EF = -0.14

FIG. A.63.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. A.64.B  DENSITY OF STATES S1, S2 AND FILLED STATES F1, F2 VS. ENERGY E. EF IS FERMI ENERGY.
FIG. B.1 FERMI ENERGY EF VS. TEMPERATURE T.
FIG. 8.2  FERMI ENERGY EF VS. TEMPERATURE T.

EF VS. T
FIG. B.4 FERMI ENERGY EF VS. TEMPERATURE T.

EF (RDB)

-1.500 -1.000 -0.500 0.000 0.500

T (K)

450.0 500.0 550.0 600.0 650.0 700.0 750.0 800.0 850.0

EF VS. T 170
FIG. C.1  SCREEN FACTOR B VS. TEMPERATURE T.
**FIG. C.2** SCREEN FACTOR B VS. TEMPERATURE T.
FIG. C.4 SCREEN FACTOR B VS. TEMPERATURE T.
Fig. D.1 Log of carrier concentration N vs. temperature T.
FIG. D.2 LOG. OF CARRIER CONCENTRATION N VS. TEMPERATURE T.
FIG. D.3 LOG. OF CARRIER CONCENTRATION N VS. TEMPERATURE T.
FIG. D.4 LOG. OF CARRIER CONCENTRATION N VS. TEMPERATURE T.
FIG. D.5 LOG. OF CARRIER CONCENTRATION \( N \) VS. TEMPERATURE \( T \).
FIG. E.1 GROUND STATE ENERGY $E$ VS. VARIATIONAL PARAMETER $A$.

$B$ is screen factor (in $1/BR$). $R$ is impurity distance (in $EP$).
FIG. E.4 GROUND STATE ENERGY $E$ VS. VARIATIONAL PARAMETER $\alpha$.
B IS SCREEN FACTOR (IN $1/\beta$). $\alpha$ IS IMPURITY DISTANCE (IN $\beta$).
FIG. E.5 GROUND STATE ENERGY $E$ VS. VARIATIONAL PARAMETER $A_1$.
$B$ IS SCREEN FACTOR (IN 1/BA). $R$ IS IMPURITY DISTANCE (IN EP)
FIG. E.7 GROUND STATE ENERGY $E$ VS. VARIATIONAL PARAMETER $A$. 
B IS SCREEN FACTOR (IN $1/BR$). $R$ IS IMPURITY DISTANCE (IN $BR$)
Fig. 8: Growth state energy vs. operational parameter R.

R1 (1/69)

E1(R1) vs. R1

E1(0) = 0.000
E1(1) = 2.000
E1(2) = 4.000
E1(3) = 6.000
E1(4) = 8.000

B = 2.10

R = 0.0
R = 0.5
R = 1.0
R = 2.0
R = 4.0

Fig. 9: Screen factor (in 1/69). R is inertia distance (in ft).
FIG. F.1 GROUND STATE ENERGY $E$ VS. VARIATIONAL PARAMETER $\alpha$.

$B$ is screen factor (in 1/BR). $R$ is impurity distance (in BR).
FIG. F.2  GROUND STATE ENERGY E VS. VARIATIONAL PARAMETER R.
B IS SCREEN FACTOR (IN 1/EP), R IS IMPURITY DISTANCE (IN EP)
Fig. 5: ODE for State Energy vs. Vertical Parameter vs.
A12 (1/101)
FIG. F.6 GROUND STATE ENERGY \( E \) VS. VARIATIONAL PARAMETER \( A \).

\( B \) IS SCREEN FACTOR (IN 1/ER). \( R \) IS IMPURITY DISTANCE (IN ER).
Fig. F.8  Ground state energy $E$ vs. variational parameter $A$. $B$ is screening factor (in $1/8pi$). $R$ is impurity distance (in $8pi$).
FIG. G.2 GROUND STATE ENERGY $E$ VS. IMPURITY DISTANCE $R$.
B IS SCREEN FACTOR (IN 1/BR).
FIG. 4
PROBABILITY P VS. THE DISTANCE R.
LOG C = 20.0, 19.0, 18.0, 17.0, 16.0, 15.0, 14.0

P VS. R

P (ARB. UNIT)
FIG. 1.1 LOG. OF LEFT SIDE OF EQ. 7-43 XF AND RIGHT SIDE FF VS. LOG. OF XF. INTERCEPT OF THE TWO IS SOLUTION OF THE EQ.
FIG. 1.2 LOG. OF LEFT SIDE OF EQ. 2-43 XF AND RIGHT SIDE FF VS. LOG. OF XF. INTERCEPT OF THE THT IS SOLUTION OF THE EQ.
FIG. 1.3 LOG. OF LEFT SIDE OF EQ. 2-43 XF AND RIGHT SIDE FF VS. LOG. OF XF. INTERCEPT OF THE TWO IS SOLUTION OF THE EQ.
FIG. 1.4 LOG, OF LEFT SIDE OF EQ. 2-43 XF AND RIGHT SIDE FF VS. LOG, OF XF. INTERCEPT OF THE TWO IS SOLUTION OF THE EQ.
FIG. 1.5 LOG OF LEFT SIDE OF EQUATION 24 versus LOG of the LOG Xf, LOG Yf.
FIG. 1.6 LOG. OF LEFT SIDE OF EQU. 2-43 XF AND RIGHT SIDE FF VS. LOG. OF XF. INTERCEPT OF THE TWO IS SOLUTION OF THE EQ.
FIG. 1.7 LOG. OF LEFT SIDE OF EQ. 2-43 XF AND RIGHT SIDE FF VS. LOG. OF XF. INTERCEPT OF THE TWO IS SOLUTION OF THE EQ.
FIG. 1.8 LOG. OF LEFT SIDE OF ED. 2-43 XF AND RIGHT SIDE FF VS. LOG. OF XF. INTERCEPT OF THE TWO IS SOLUTION OF THE ED.
APPENDIX B

COMPUTER PROGRAM
MAIN PROGRAM: PRESENT CONSTANTS ARE FOR PHOSPHORUS IN SILICON.

SUBROUTINE SFE (A, B, C, D) PLOT S1, S2, F1, F2 VS. F, WHERE A, B, C ARE INITIAL, FINAL AND STEP VALUES FOR LOGARITHM OF IMPURITY CONCENTRATION. D IS TEMPERATURE IN KELVIN. D IS AT 1.0, 6.

EXECUTION TIME: ABOUT 3 SECONDS PER CONCENTRATION PER TEMPERATURE.

SUBROUTINE EF8N (A, B, C, D) PLOT E, F, N VS. 1, WHERE A, B, C ARE DEFINED AS BEFORE. ALL CONCENTRATIONS ARE PLOTTED ON 1 GRAPH. EXECUTION TIME: ABOUT 1 MINUTE PER CONCENTRATION.

SUBROUTINE FXF (A, B, C, D) PLOT GRAPHICAL METHOD WHICH DETERMINES EF, WHERE A, B, C, D ARE DEFINED AS BEFORE. IF D IS LESS THAN 6., 1 GRAPH IS MADE FOR TEMPERATURES 10, 20, 40, 60, 160, 320. EXECUTION TIME: ABOUT 10 SECONDS PER CONCENTRATION PER TEMPERATURE.

SUBROUTINE PRC (A, B, C) PLOT P VS. R, WHERE A, B, C ARE DEFINED AS BEFORE. ALL CONCENTRATIONS ARE PLOTTED ON 1 GRAPH.

SUBROUTINE EAA (E, F, G, H) PLOT E1(A), E12(A) VS. A, WHERE E, F, G ARE INITIAL, FINAL AND STEP VALUES FOR BETA, H IS DISTANCE IN BURR RADIUS. IF H IS LESS THAN 0., 1 GRAPH IS MADE FOR DISTANCES 0, .5, 1, 2, .4, 8.

SUBROUTINE EAR (E, F, G) PLOT E1, E12-E1, A1, A12 VS. P, WHERE E, F, G ARE DEFINED AS BEFORE. ALL BETAS ARE PLOTTED ON 1 GRAPH.

SUBROUTINE PER (A, B) PLOT PROBABILITIES. GROUND STATE ENERGY VS. IMPURITY DISTANCE FOR 10 TO 10^7 POWER CONCENTRATION, B DEGREE K.

EXECUTION TIME: 5 SECONDS.

COMMON /MBK/ RMC, RPE, RKE, ED, RB, RNO, BN, PI
COMMON /ICBK/ T(10), C, CS

T(1) = 10.
T(2) = 20.
T(3) = 40.
T(4) = 60.
T(5) = 100.
T(6) = 200.
T(7) = 300.
T(8) = 400.
C = 16.
CS = .5.
RMC = 6.
RPE = .327.
RKE = 11.8.
ED = .44.
RB = .26.
RNO = 482957E16.
BN = 209983E-1.
PI = 3.14159.
DO 20 1 = 1, 8.
XC = C + 5*FLOAT(1-1).
DO 30 J = 1, 8.
CALL PFR (XC,T(J))
20 CONTINUE
20 CONTINUE
STOP
END

C PLOT S1,S2,F1,F2 VS. E WITH C,T AS PARAMETERS
SUBROUTINE SFE (C1,CIF,CIS,TEMP)
REAL K3(3), E12(2,2,2), A12(2,2,251), S12(2,251), F12(2,251)
REAL XP(251),YP(251)
COMMON /MBK/ RNC,RNE,RKE,ED,RB,END,BO,PL
COMMON /FBK/ CR,RTT,CB,T
COMMON /RTBK/ XC,T1
COMMON /ICBK/ TG(10)
A1D=ALOG (10.)
K=251
IF (TEMP .LT. 6.) TEMP=6.
T=TEMP
N=1
DO 400 I=1,K
XP(I)=.02*FLOAT(I-201)
400 CONTINUE
IF (C1 .EQ. 0.) C1=.5
NS=FIX((CIF-C1)/C1-.1))
70 91 IC=1,NS
C=CIF*FLOAT(IC-1)*C1
C=1D.**XC
DO 20 N=1,8
IF (T .EQ. TG(N)) GO TO 30
20 IG=(IC-1)*8+N
FG=FLOAT(CG)
CALL PLOT1 ('S1,S2,F1,F2 VS. E (RDB)')
C'S1,S2,F1,F2 (ARB. UNIT)
CALL PLOT1 (5,-7,-3)
CALL PLOT3AX (0.,0.,5.)
CALL PLOTGM (-4.,-5.,1000.,3)
CALL SYMBOL (1.8,9.2,1.,0.,0.6)
CALL NUMBER (999.,999.,1.,0.,1.)
CALL SYMBOL (1.9,9.2,1.,0.,0.2)
CALL NUMBER (999.,999.0,1.,T,0.,-1)
CALL SYMBOL (1.9,9.2,1.,EF=4.,0.,3)
RKT=.08617/T/EN
RNC=RND*RNC*SQRT(RME*T)**3
CC=C/RNC
CB=C*RNC**3
CR=C8@4.*PI/3.
CALL FNRT(R3,IR)
DO 5 I=1,IR-2
   EF=R3(I)*4*ROKTY
   CALL NUMBER (999.0,999.0,1,EF,0.,2)
   CALL SYMBOL (999.0,999.0,1,EF,0.,2)
5 CONTINUE
   DO 10 IP=1,10,2
      XF=10.*R3(IP)
      D=SQRT(AD+RNO*RMQ+SQRT(RME)*3*SQRT(1)+5*HF(XF)/RKE)*R
      CALL EKB(E12,A12,E)
   DO 65 J=1,2
      SIZ(J,1)=0.
      F12(J,1)=0.
65 CONTINUE
   DO 66 J=1,2
      E12(1,42)=.5*(E12(1,41)+E12(2,41))
      E12(2,42)=E12(1,42)
   DO 119 J=1,2
      A2=1.
      AC=0.
   DO 120 I=1,42
      R=-2*(FLOAT(I)*.5).
      A1=A2
      E1=E2
      E2=E12(J,1)
      TM=CR*R**3
      DX=ABS(E2-E1)
      IF (DX.42) DX=.22
      IF (TM.61.90.) GO TO 150
      IF (I.EQ.42) GO TO 150
      A2=EXP(-TM)
   GO TO 160
119 CONTINUE
120 CONTINUE
150 A2=0.
160 AL=AC
   AC=(A1-A2)/DX
   AFL=AC
   Y=E12(1,1)/RKT
   IF (Y.61.-90.) GO TO 180
   Y1=.5*EXP(-90.)/XF
   GO TO 190
180 Y1=.5*EXP(Y)/XF
190 Y=E12(2,1)/RKT
   IF (Y.61.-50.) GO TO 200
YS = 1.75*B*ALOG10 (YP(152)/3).
CALL SYMBOL (XS,YS,.1,52*,0.,2)
DO 430 I = 1,K
YP(1) = F12(1,1)
IF (YP(1) .LT. 1.) YP(1) = 1.
CONTINUE
CALL PLUP (XP,YP,X(1),0,
XS = 1.5*6.*(XP(IS1M4.1/5.-.4)*5*I/.75*B*.ALQG10(IYPCI\11/3.
CALL SYMBOL (XS,YS,.1,*F1*,0.,2)
DO 440 I = 1,K
YP(1) = F12(2,1)
IF (YP(1) .LT. 1.) YP(1) = 1.
CONTINUE
CALL PLUP (XP,YP,X(1),0,
XS = 1.5*6.*(XP(IS2M4.I/5.-.2)*5*4.2
YS = 1.75*B*.ALOG10(YP(IS2))/3.
CALL SYMBOL (XS,YS,.1,*.F2*,0.,2)
CONTINUE
CALL SYMBOL (1.5,.1,.1,*F1*,.0.,7)
CALL Number (999.0,999.0,.1,.0,-1)
CALL SYMBOL (999.0,999.0,.1,.0,.B DENSITY OF STATES S1,S2 AND FILL CED STATES F1,.0,.5)
CALL SYMBOL (1.5,.8,.1,*F2* VS. ENERGY E. EF IS FERMI ENERGY,.0.,
Continued
CALL PLOT.
91 CONTINUE RETURN
END

C PLOT EF,B,N VS. T WITH C AS PARAMETER
SUBROUTINE EFBN (C11,C1F,C1SI
REAL P3(3),EF(3,101),B(3,101),N(3,101),X(101),Y(101)
REAL YN(3),YX(3),LB(3,1000)
INTEGER NN(50)
COMMON /MBK/ RMC,RK,RK,E,ED,RP,RND,AD,P1
COMMON /FBK/ CR,RK1,CC,1
COMMON /TBK/ XC,11
A10 = ALOG(10.)
IF (CIS .Eq. 0.) CIS = .5
NS = IFIX((CIF-CIS)/CIS+.1)
L = 0
N1 = 0
YN(1) = 0.
YX(1) = -10.
YN(2)=5.*
YN(3)=20.*
YX(1)=0.*
YX(3)=0.*
NT=62
DO 10 IC=1,NS
XC=CT1+FLOAT(IC-1)*C1S
C=10.*+XC
II=1
I2=0
DO 20 IT=1,NT
T=2.*FLOAT(IT+2)
IF (IT .GT. 28) T=10.*FLOAT(IT-28)+60.
IT=IT+1
10 CONTINUE
RKT=.08677*Y/ED
RNC=RND*RMC*SQRTRME*T**3
CC=C/RNC
CB=C070003
CR=CB**.0PI/3.
IF ((IT .GT. 60.) .OR. (XC .LT. 17.5)) GO TO 11
CALL FNRT (R3,IR)
GO TO 12
11 IR=1
R3(1)=RNDT(1-20.,5.)
12 DO 30 I=1,IR,2
EF(I,IT)=R3(I)*AI0+KKT
XK=10.*R3(I)
&G(I,IT)=SQRTRD(RKO*RND*RMC*SQRTRME**3*SQRFTT*SPF/XF)/PE*RK
TN=RNC*XK*SM(XF)
CN(I,IT)=ALG10 (AMAXI (1.,TN))
30 CONTINUE
IF (IR .EQ. 1) II=0
IF (IR .GT. 1) 12=12+11
20 CONTINUE
IP=1
IF (12 .GT. 1) IP=3
H=NT
DO 40 I=1,IP,2
IF (I .GT. 1) N=12
L=L+1
MV(I)=N+1
40 DO 50 J=1,N
J1=41+J
EBC(I,J1)=EF(I,J)
EBC(2,J1)=Bo(I,J)
EBC(3,J1)=CN(I,J)
50 CONTINUE

IF (YN(I)) EQ EBC(I,J) YN(I)=EBC(I,J)
IF (YN(I)) EQ EBC(I,J) YN(I)=EBC(I,J)
IF (YN(I)) EQ EBC(I,J) YN(I)=EBC(I,J)
IF (YN(I)) EQ EBC(I,J) YN(I)=EBC(I,J)
IF (YN(I)) EQ EBC(I,J) YN(I)=EBC(I,J)
IF (YN(I)) EQ EBC(I,J) YN(I)=EBC(I,J)
IF (YN(I)) EQ EBC(I,J) YN(I)=EBC(I,J)

50 CONTINUE
N=N+1
40 CONTINUE
10 CONTINUE
IF (L.LT. 1) GO TO 200
DO 210 I=1,3
YI=0.
IF (I1 .LE. 2) YI=.5
SGN=1.
IF (YN(I)) .LT. 0.) SGN=-1.
YMAX=FLOAT(IFIX(YN(I)+SGN*Y.I))
IF (YMAX .LT. YN(I)) YMAX=YMAX+(1.-YI)
SGN=1.
IF (YN(I)) .LT. 0.) SGN=-1.
YMIN=FLOAT(IFIX(YN(I)+SGN*Y.I))
IF (YMIN .GT. YN(I)) YMIN=YMIN-(1.-YI)
IF (YMAX-YX(I)) .LT. 0.) YMAX=YMAX+(1.-YI)
IF (NO .LE. 2) ND=.5
IF (NO .LE. 3) GO TO 130
DO 140 IN=3,9
IF (MOD(NO,IN) .NE. 0) GO TO 140
ND=IN
150 CONTINUE
140 CONTINUE
NO=NO+1
130 IF (T3 .NE. 1) GO TO 211
CALL PLOTL ("EF VS. T", T(K),"EF (RDB)"
GO TO 220
211 IF (T3 .NE. 2) GO TO 212
CALL PLOTL ("B VS. T", K,"B (IV)"
GO TO 220
212 CALL PLOTL ("LOG N VS. T", K,"LOG N"
220 CALL PLOT (5,9,-3)
CALL PLOTMAX (0.0,0.85)
CALL PLOTSIG (0.0,0.4, YMIN, YMAX, ND)
IF (T3 .NE. 1) GO TO 300
CALL SYMBOL (1.3,1.,"FIG. FERMI ENERGY FF VS. TEMPERATURE")
SCREEN FACTOR B VS. TEMPERATURE

LOG. CF CARRIER CONCENTRATION N

C PLOT F(XF) VS. XF WITH L,1 AS PARAMETERS
SUBROUTINE FXF (C11,C1F,CIS,TFMP)
COMMON /FBK/ RMC,RKF,RKE,ED,RNP,BO,PI
COMMON /F BK/ CR,RTK,CC,T
COMMON /RTBK/ XCI,T1
REAL R3(3), XP(201),YP(201)
LOGICAL TSET
AID=ALOG(10.)
46=.6
:SET=.FALSE.
IF (ICMP .GE. 6.) :SET=.TRUE.
IF (:SET) N6=1
IF (CIS .EQ. 0.) CIS=.5
NS=10**((C1F-C11)*(C1S+I.7))
DO 91 IC=1,NS
XC=C11+FLOAT(IC-1)*C15
C=10.*XC
DO 200 J=1,101
XP(J)=FLOAT(J-81)**.25
CONTINUE
200 CONTINUE
CALL PLSTYL 1' $',*LOG XF.(OR EF/2.3KT)*',*LOG XF,LOG FF$'
CALL PLOT (.9,.9,-3)
CALL PLOTSAX (0,0.5,.5)
CALL PLTRSM (-20,.5,.5,-20,.5,.5)
CALL PLTRFY (XP,XP,101,1,0)
CALL SYMBOL (2.8,.9,.9,.13,*LOG XF,LOG FF VS. LOG XF',0.,.24)
CALL SYMBOL (1.9,.9,.9,.1,*LOG C=.1,.O,.6)
CALL NUMBER (999,0,999,0,.1,XC,0,.1)
CALL SYMBOL (1.5,1,1,'LOG. OF LEFT SIDE OF EQ. XF
C AND RIGHT SIDE FF;0.,.60)
CALL SYMBOL (1.5,.8,.1,VS. LOG. OF XF. INTERCEPT OF THE TWO IS SO
CLUTION OF THE EQ. XF)
DO 90 IT=1,NS
T=10.*2.**([IT-1)
IF (ITET) T=TEMP
IT=1
RK1=0.617*T/EO
RNC=RNO*RNC*SQRT(HE*T)**3
CC=C/RNC
CB=CS/RNC
CR=CB**.9.*PI/3.
DO 300 IX=1,101
YP(IX)=YP(IF(IX))
IF (YP(IX) LT -20.) YP(IX)=-20.
IF (YP(IX) GT 5.) YP(IX)=5.
CONTINUE
300 CONTINUE
N=82+IFIX(XC*2.)
YT=1.75+8.*(YP(N)+20.1)/25.2-.045
XT=1.5*6.2*(XP(N)+20.)/25.2-.045
CALL PLTRSM (XP,YP,101,1,0)
CALL SYMBOL (XT,YT,.09,.09,.0,.0,.2)
CALL NUMBER (999,0,999,0,.09,1,0,.1)
90 CONTINUE
CALL PLOT1ON
91 CONTINUE
RETURN
END
C PLOT P VS. R WITH C AS PARAMETER
SUBROUTINE PRC (C1, C2, C3)
EXTERNAL PR
COMMON /RH/ RMC, RPE, RKE, E0, R0, RNO, ROI, PI
COMMON /RK/ CR
REAL XC(20)
IF (C1 .EQ. 0.) C1 = .5
NS = IFIX((C2 - C1) / C3)
CALL PLOT ('P VS. R$^*$, 'R (BR) $^*$', 'P (ABD. UNIT)$^*$')
CALL PLOT (.5, .7, -3)
CALL PLOT (.0, .0, .85)
CALL PLOT (.0, .4, .0, 1, .5)
CALL SYMBOL (1.5, 1.5, 1., 'FIG. P(RES. P VS. IMPURITY DISTANCE')
CCE R$, .0, .47)
CALL SYMBOL (1.5, .8, .1, FROM LEFT TO RIGHT :*, 0, .20)
DO 10 IC = 1, NS
   IC = NS - IC-1
   XC(ICI) = C1 + FLOAT(ICI) * C2
   C = 10.**XC(ICI)
   CR = C * RMC**3 * A + PI/3.
   CALL PLOT (0., 0., PR, 0)
10 CONTINUE
CALL SYMBOL (1.5, 1.5, 1., LOG C = *, .0, .6)
CALL NUMBER (999.0, 999.0, 0., 1, XC(1), 0., 1)
IF (NS .LT. 2) GO TO 30
DO 20 I = 2, NS
   CALL SYMBOL (999.0, 999.0, 0., 1, *, 0., 1)
   CALL NUMBER (999.0, 999.0, 0., 1, XC(1), 0., 1)
20 CONTINUE
30 CALL PLOTS
RETURN
END

C PLOT E(A) VS. A WITH B, R AS PARAMETERS
SUBROUTINE EAA (B1, B2, NS, DIST)
REAL X(200), Y(200), F12(2000)
LOGICAL RSET
COMMON /EEAK/ U, BC, B2
NS = 5
RSET = .FALSE.
IF (DIST .GE. 0.) RSET = .TRUE.
IF (RSET) NS = 1
IF (RSET .EQ. 0.) RSET = 2
NS = IFIX((B2 - B1) / NS + 1.1)
DO 100 I = 1, 121
100  X(I) = 0.2*FLOAT(I-1)
    CONTINUE
    DO 50  I=1,NS
      B=0.1+FLOAT(I-1)*BS
      DO 30  J=1,2
        YX=0.
        YN=0.
        IF (J .GT. 1) GO TO 110
        CALL PLOTL (' ', 'A1 (1/BR)', 'E1(A1) (KDB)', '')
        GO TO 120
      110 CALL PLOT (' ', 'A12 (1/BR)', 'E12(A12) (KBR)', '')
      120 CALL PLOT (' ', 'A12 (1/BR)', 'E12(A12) (KBR)', '')
      DO 10  IR=1,N6
        R=0.5*2.**(IR-2)*AMIN1(FLOAT(IR/2),1.)
        IF (RSET) R=DIST
        U=R/R
        BE=EXP(-U)
        IF (U .GT. 2) GO TO 5
        GO TO 6
      5  B2=(1.-BE-U)/U/V
      6  DO 20  J=1,121
        JI=2*(IR-1)+J
        E12(JI)=EE(1.X(J),R,B)
        IF (YX .LT. E12(JI)) YX=E12(JI)
        IF (YN .LT. E12(JI)) YN=E12(JI)
      20 CONTINUE
    10 CONTINUE
    YMAX=FLOAT(IFIX(YX))
    IF (YMAX .LT. YX) YMAX=YMAX+1.
    YMIN=FLOAT(IFIX(YN))
    IF (YMIN .LT. YN) YMIN=YMIN-1.
    NY=1+FIX(YMAX-YMIN)
    IF (NY .LT. 2) NY=4
    IF (NY .LT. 8) GO TO 60
    70 DO 80  IN=3,9
    IF (MOD(NY,IN) .NE. 0) GO TO 80
    NY=IN
    GO TO 60
CONTINUE
NY=NY+1
YMAX=YMAX+1.
GO TO 70
60 CALL PLOTSGN (0.,3.,3,YMIN,YMAX,NY)
IF (1.,.GT. 1) GO TO 200
CALL SYMBOL (3.6,9.9,.13,'E1(A1) VS. A1',0.,13)
GO TO 210
200 CALL SYMBOL (13.4,9.9,.13,'E12(A12) VS. A12',0.,16)
210 CALL SYMBOL (1.8,1.,'B IS SCREEN FACTOR (IN I/BR). R IS IMPURITY DISTANCE (IN BR)',0.,60)
DO 130 IR=1,6
R=.5*2.*AMIN1(FLOAT(IR/2),1.)
IF (RSET) R=0ST
DO 140 J=1,121
Y(J)=E12(J)
140 CONTINUE
CALL PLSPT (X,Y,121,1,0)
XS=1.5*6.*X(121)/3.+0.5
YS=1.75*8.*Y(121)-YMIN/(YMAX-YMIN)-.05
CALL SYMBOL (XS,YS,'R=0.0,.2)
CALL NUMBER (999.0,999.0,1,R,0.,1)
130 CONTINUE
CALL PLSQN
30 CONTINUE
50 CONTINUE
RETURN
END

C...PLOT E:A VS. B WITH B AS PARAMETER
SUBROUTINE EAR (BI,BF,RS)
REAL E12(2,42),A12(2,42),EA(4,820),X(42),Y(42)
REAL YMAX(4),YMIN(4)
YMIN(1)=-4.
YMAX(1)=1.
YMIN(2)=-2.
YMAX(2)=.5
YMIN(3)=-.5.

223
VMAX(3) = 2.
VMIN(4) = 0.5
VMAX(4) = 2.
MD = 5
DO 5 I = 1, 141
   X(I) = 2*FLOAT(I-1)
   CONTINUE
   IF (AS .EQ. 0.1  AS = 0.2
   NS = IFIX((BF - BI)/BS + 1.1)
   DO 10 I = 1, NS
   B = BI*FLOAT(I - 1)*BS
   CALL ERB (E12, A12, B)
   DO 20 J = 1, 41
   J1 = (I - 1)*41 + J
   EA(1, J1) = E12(1, J)
   EA(2, J1) = E12(2, J)
   EA(3, J1) = AI2(1, J)
   EA(4, J1) = AI2(2, J)
   20 CONTINUE
   CONTINUE
   DO 30 I = 1, 4
   IF (I .GT. 1) GO TO 100
   CALL PLOTSL ('E1 VS. R$, 'R (BR)$$, 'E1 (RDB)$')
   GO TO 130
   100 IF (I .GT. 2) GO TO 110
   CALL PLOTSL ('E2(-L2 - E1) VS. R$, 'R (BR)$', 'E2 (RDB)$')
   GO TO 130
   110 IF (I .GT. 3) GO TO 120
   CALL PLOTSL ('A12 VS. R$, 'R (BR)$', 'A12 (1/BR)$')
   GO TO 130
   120 CALL PLOT (3.8, 6.8, -3)
   CALL PLOTS (0.0, 0.0, 0.85)
   CALL PLOGM (0.0, 0.4, VMIN(I), VMAX(I), ND)
   IF (I .GT. 2) GO TO 300
   CALL SYMBOL (1.5, 1.5, 'FIG.  GROUND STATE ENERGY E VS. IMPURITY DISTANCE R$$.85$')
   GO TO 310
   300 CALL SYMBOL (1.5, 1.5, 'FIG. VARIATIONAL PARAMETER A VS. IMPURITY DISTANCE R$$0.85$$')
   GO TO 310
   310 CALL SYMBOL (1.5, 0.8, 'B IS SCREEN FACTOR (IN 1/BR) .', '0 .29')
   DO 40 J = 1, NS
   DO 50 K = 1, 141
   K1 = (J - 1)*41 + K
Y(1) = EA(I, K1)

CONTINUE
CALL PLTSP (X, Y, 1, 1, 0)
YSH = 0.05
IF (J.EQ. 1) YSH = 0.05 + FLOAT(I/3) * 0.05
IF (J.EQ. NS) YSH = 0.05 + FLOAT((5-I)/3) * 0.05
X$ = 1.5 + 15
YS = 1.55 + 0.05 * (Y(1) - YMIN(1)) / (YMAX(1) - YMIN(1)) + YSH
FAC = 1.0 / (YMAX(1) - YMIN(1))
SL = (Y(4) - Y(2)) / (X(4) - X(2)) * FAC
ANG = ATAN(SL) * 180. / 3.14159
B = BI * FLOAT(J-1) * BS
CALL SYMB (XS, YS, 0.05, "B", ANG, 2)
CALL NUMBER (999.0, 999.0, 0.09, B, ANG, 2)

CONTINUE
CALL PLTSDN

CONTINUE
RETURN

END

C PLOT P, E1, E2 VS. R FOR GIVEN CONCENTRATION AND TEMPERATURE
SUBROUTINE PER (XC, T)
EXTERNAL EP
COMMON /NBK/ RMC, RME, RKE, ED, RB, RNO, BO, PI
COMMON /FBK/ CR
COMMON /TCBK/ TGHO, CI, C5
REAL BETA(3), EF(3), X(50), Y(50), E12(2, 50), A12(2, 50)
DO 20 N = 1, 8
IF (T.EQ._T(G(N))) GO TO 30
20 CONTINUE
30 IC = IFIX ((XC- CI) / CS + 1)
IG = IC + N
E2 = FLOAT(IG)
DO 5 I = 1, 41
X(I) = -2.4 * FLOAT(1-I)
Y(I) = 0.
5 CONTINUE
CALL BCT (XC, T, BETA, EF, IR)
CALL PLTSTL ("P, E1, E2 VS. RS", "R (BR)"*
C "E1, E2 (RDB), P (ARB, UNIT)"
CALL PLOT (5, 5, -3)
CALL PLTSAX (3, 0.0, 0.05)
CALL PLTSGM (0.0, 0.5, 4.0, -4.0, 5)
CALL SYMB (1.5, 1.1, "FIG, A", 0.0, 1)
CALL NUMBER (999.0, 999.0, 0.09, 0, 0, 1)
CONTINUE
CALL PLTSON
RETURN
END

LOG F(X)
FUNCTION YF (X)
REAL E12(2,42),A12(2,42)
COMMON /MBK/ RHC, RYE, RKF, ID, RHO, RHO, PI,
COMMON /FBR/ CR, RKT, CC, T,
XF=10.**X
S=SQR1(B0*KH1)RMC*SQR1(RM1)**3*SQR1(7)**3MP(XF)/RKE**RKE
CALL ERB(E12,A12,0)
S=0.
AC=1.
30 30 I=2,41
P=2*FLOAT(I-1)
AL=AC
TH=CR*R**3
IF (TH .GT. 90.) GO TO 35
AC=EXP(-TH)
GO TO 36
35 AC=0.
36 A=AL-AC
Y=E12(I,1)/RKT
IF (Y .GT. -90.) GO TO 45
Y1=.5*EXP(-90.)/XF
GO TO 46
45 Y1=.5*EXP(Y)/XF
46 Y=E12(2,1)/RKT
IF (Y .GT. -90.) GO TO 55
Y2=.5*EXP(90.)/XF
GO TO 56
55 Y2=.5*EXP(-Y)/XF
56 S=S*(1.0+Y1+Y2)
60 CONTINUE
Y=-5*(E12(1,1)+E12(2,1))/RKT
IF (Y .GT. -90.) GO TO 100
Y1=.5*EXP(-90.)/XF
Y2=.5*EXP(90.)/XF
GO TO 110
100 Y1=.5*EXP(Y)/XF
Y2=.5*EXP(-Y)/XF
110 S=S*AC*(1.0+Y1+Y2)
F=CC*S/SM(XF)
VF=ALOG10(F)
RETURN
END

C  FIND ROOT FOR F(X) = X

FUNCTION ROOT (XL, XR)

COMMON /YBK/ YC, Y
LOGICAL YLGXL
XL=AMIN(XL, XR)
XR=AMAX(XL, XR)
YL=YF(XL)
YR=YF(XR)

IF (((YL-XL)*(YR-XR)) .GE. 0.) GO TO 70

IF (YL .LT. XR) GO TO 100

XL1=XL

DO 110 I=1, 3, 2
XL=XL1+.E-4*FLOAT(I-1)
YL=YF(XL)

IF (((YL-XL)*(YR-XR)) .LT. 0.) GO TO 200

110 CONTINUE

XN=XL
GO TO 20

100 IF (YL .GE. XR) GO TO 200

XR1=XR

DO 120 I=1, 3, 2
XR=XR1+.E-4*FLOAT(I-1)
YR=YF(XR)

IF (((YL-XL)*(YR-XR)) .LT. 0.) GO TO 200

120 CONTINUE

XN=XR
GO TO 20

200 YLGXL=.FALSE.

IF (YL .LT. XR) YLGXL=.TRUE.

D=AMIN1(ABS(YL-XL),ABS(YR-XR), .01)

DO 150 I=1, 50
XN=.5*(XL+XR)

IF (ABS(XL-XR) .LE. .01) GO TO 20

SL=(YL-YR)/(XL-XR)

IF (SL .LE. 1.) GO TO 20

XN=(YL-SL*XR)/(1.-SL)

IF (MOD (I, 2) .EQ. 0) XN=.5*(XL+XR)

YN=YF(XN)

IF (ABS (YN-XN) .LE. .01) GO TO 20

IF (MOD (I, 2) .EQ. 1) D=AMIN1 (ABS(YR-XN), .01)

IF (YN .GE. XR) GO TO 30

IF (YLGXL) GO TO 10 40

XL=XR
YL=YN
GO TO 10
XR=XN
YR=YN
GO TO 10
IF (YLGXL) GO TO 50
XR=XN
YR=YN
GO TO 10
50 XL=XN
YL=YN
10 CONTINUE
70 PRINT 60,XL,YL,RR,TR,XC,1
60 FORMAT (1X,'IF FAIL TO FIND ROOT BETWEEN (','F6.2',';',F6.2,') /1X,'AT LOG C=','F4.1',' T=','F4.0')
20 ROOT=XN
RETURN
END

C FIND 3 ROOTS FOR F(x)=y II FAIL II
SUBROUTINE FNRT (F?,IP)
REAL F3(3),G0(3)
IP=1
F3(1)=F0RT(-20.,5.)
YL=F3(1)
IF (YI .GT. 0.) GO TO 10
IF (YI .LT. -5.) XI=-5.
30 XP=YI+.7
IF (YI .GT. 5.) GO TO 10
IF (YF(XR) .GE. YF) GO TO 20
SL=(YF(XR+.05)-YF(XF-.05))/.1
XL=XF
IF (SL .LT. 1.) GO TO 20
40 XP=XL+.7
IF (XF .GT. 5.) GO TO 10
IF (YF(XR) .GE. YF) GO TO 20
SL=(YF(XR+.05)-YF(XP-.05))/1.
IF (SL .LT. 1.) GO TO 20
YL=XF
GO TO 40
50 GO TO 1,6
XR=YF(YR+YL)
IF (YF(YR) .LT. XR) GO TO 70
XR=XN
GO TO 20

SL = (YF(XN + .5) - YF(XN - .5)) / .1
IF (SL .LT. 1.) GO TO 110

YL = YN
GO TO 60

60 CONTINUE
GO TO 90

20 R(2) = FDOT(XL, XP)
R(3) = FDOT(XR, YL)
GO TO 100

10 X' = F(1)
IF (X' .LT. -1.) GO TO 90

130 Y' = X' / 7.
IF (Y' .LT. -5.) GO TO 90
IF (YF(Y') .LE. YL) GO TO 120
SL = (YF(XL + .5) - YF(XL - .5)) / .1
XP = XL
IF (SL .LT. 1.) GO TO 110

140 XL = YP * .7
IF (X' .LT. -5.) GO TO 90
IF (YF(Y') .LE. YL) GO TO 120
SL = (YF(XL + .5) - YF(XL - .5)) / .1
IF (SL .LT. 1.) GO TO 110
XP = XL
GO TO 160

150 IF (I = 1.) I = 1.5
YN = .5Y(YR + XL)
IF (YF(YN) .GT. XN) GO TO 170
YL = YN
GO TO 120

170 SL = (YF(YN + .5) - YF(YN - .5)) / .1
IF (SL .LT. 1.) GO TO 160

XR = YN
GO TO 160

160 CONTINUE
GO TO 90

120 R(2) = FDOT(XL, XP)
R(3) = FDOT(XR, YL)
100 IF = 3
R'MAX = R(1)
THAY = 1
ND 200. 1 = 7, 3

230
TF (RMAX .GE. R3(1)) GO TO 200
RMAX=R3(1)
I.MAX=1
200 CONTINUE
J=1
DO 210 I=1,3
IF (1 .EQ. I.MAX) GO TO 210
J=J+1
RD(J)=R3(1)
210 CONTINUE
R3(1)=RMAX
R3(2)=AMAX1(RD(2),RD(3))
R3(3)=AMAX1(RD(2),RD(3))
90 RETURN
END

C E1,E2,A1,A2 AS A FUNCTION OF R,B

SUBROUTINE ERB (E12,E12,BS)
REAL E12(2,42),A12(2,42)
R=ABS(RS)
B1=AMAX1(FLOAT(IFX(B)/5),1.)
DO 10 1=1,2
A=(2.-FLOAT(11)-1.)*5./16.)*(1.-B/5.)*(1.-B1)
IF (A .LT. -.1) A=-.1
DO 20 J=1,41
AL=A
R=.2*FLOAT(J-1)
CALL AVE (AN,EM,1,A,R,B).
A12(1,J)=AM
A=AM
XE=E12(J,1)+FLOAT(1-1)
E12(J,1)=EM-XE
IF (.NOT. (J .NE. 1)) A=2.*A-AL
20 CONTINUE
10 CONTINUE
RETURN
END
C FIND VALUE OF A WHICH MINIMIZE E

SUBROUTINE AME(AH, EM, A, RS, BS)
COMMON /EBK/ U, R, A
REAL E(3), AS(5), AP(100), EP(100)

B = ABS(RS)
R = ABS(R)
A = ABS(A)
NA = 0

U = B * R
IF (U .GT. 50.) GO TO 40
BE = EXP(-U)
GO TO 30

40 BE = 0.

50 IF (U .GT. 2) GO TO 5

GO TO 6

5 B2 = (1. - BE - U) / U * 2
6 DO 11 ID = 1, 100

AT = A

AP(10) = A
DO 30 M = 1, 3
A = AT + 0.08 + (FLOT(M) - 2.1)

E(M) = EF(1, A, R, B)

30 CONTINUE

EP(10) = E(2)
OX = E(1) - 2.4 * E(2) + E(3)
IF (OX .LT. 0.01) OX = 0.01
A = AT + 0.04 + (E(1) - E(3)) / OX
DO 60 K = 1, 10
IF (ABS(A - AP(K)) .GT. 0.02) GO TO 60
NA = NA + 1

IF (NA .GE. 3) GO TO 31

AS(NA) = A

60 CONTINUE

11 CONTINUE

DO 12 J = 1, 20
PRINT 13, B, R, AP(J), EP(J)

13 FORMAT(1X, 9.4, 9.3X, 9.3X, 9.3X, 9.3X, 9.3X, 9.3X, 9.3X, 9.3X, 9.3X)
12 CONTINUE

PRINT 14

14 FORMAT(1X, *A NOT CONVERGING!

31 AH = (AS(1) + AS(2) + A) / 3.
EM = EF(1, A, R, B)
RETURN
END
C PROCESS IN CALCULATION OF E12

FUNCTION EE (I, A1, U, B1)
COMMON /EEDK/ U, B, E, R
A = ABS(A1)
B = ABS(B1)
R = ABS(R1)
IF (A .NE. 0.) GO TO 5
EE = 0.
GO TO 26
5 AA = A * A
H = A / (A + 0.5) * B
HH = H + H
W = A + R
WW = W * W
IF (R .EQ. 0.0) GO TO 10
H3 = W * H
IF (H .GT. 50.) GO TO 40
AX = EXP(-W)
GO TO 50
40 AX = 0.
50 Y = 2. * W - U
YY = Y * Y
S = AX * (1. + W + H3)
SK = S - 2. * AX + H3
IF (YY .GT. .25) GO TO 15
GO TO 60
15 IF (Y .GT. 50.) GO TO 60
EY = EXP(-Y)
GO TO 70
60 EY = 0.
70 YY = 1. - EY + Y * 5 * YYYY / 6.
6. / YYYY
16 Y3 = Y + Y4 + 1. / 6.
Y2 = Y * Y3 + .5
Y1 = Y * Y2 + .5
EE = (A * (1. + SK) + A * (2. * RK - HH * RJ)) / (1. + 5)
GO TO 25
RJP = EE * (HH + TM * HH * HH * HH * HH * HH * HH * (H + 2. * H + Y3 + 2. * HH + 4)
G = ABS(5. * B / A)
K = IFIX(G)
D=E-FLOAT(K)
SSM=SM(K,W,H)*(1-D)
SSM=SM*SUM(K+1,W,H)*D
RKP=-S*HH*(.5+HH)AX+AX*(1+*SM
FE=(2*AA*(1.5*SK)+AX*(2.4RR)-4.*HH+RJP+.5*RK+RKP))/((1.+S*5)
GO TO 26
10 FE=FLOAT(I)*(AA-4.*A*HH)+(FLOAT(I)-1.)*.5*A*HH+(.5+HH)
26 RETURN
END

C FERMI INTEGRAL

FUNCTION SM(E)
SM=0.
R4=4.
DO 10 I=1,100
X=1*FLOAT(I)
SM=SM+R3+SQR0(XI/(E+EXP(X)))
R4=R4-R4
10 CONTINUE
PI=3.14159
SM=SM*2/SQR0(P1)/3.
RETURN
END

C FERMI INTEGRAL -NEXT ORDER

FUNCTION SMP(E)
SMP=0.
R3=4.
DO 10 I=1,100
X=1*FLOAT(I)
TM=EXP(X)
SMP=SMP+R3*SQR0(TM)/(E+TM)**2
R3=R3-R3
10 CONTINUE
PI=3.14159
SMP=SMP*E*2/SQR0(P1)/3.
RETURN
END
C PROCESS IN CALCULATION OF KSP

FUNCTION STM (K,H,WW)
IF (K .GE. 16) GO TO 160
IF (K .GE. 8) GO TO 80
IF (K .NE. 0) GO TO 10
STM=2.00243*H*1.50709*WW*.55466*W*WW*.01456
GO TO 300
10 IF (K .NE. 1) GO TO 20
STM=2.00196*H*1.56891*WW*.51171*W*WW*.01426
GO TO 300
20 IF (K .NE. 2) GO TO 30
STM=2.00011*H*1.55493*WW*.46202*W*WW*.01722
GO TO 300
30 IF (K .NE. 3) GO TO 40
STM=1.99791*H*1.55490*WW*.41181*W*WW*.07403
GO TO 300
40 IF (K .NE. 4) GO TO 50
STM=1.99577*H*1.55152*WW*.3642*W*WW*.02712
GO TO 300
50 IF (K .NE. 5) GO TO 60
STM=1.99391*H*1.54822*WW*.32063*W*WW*.02795
GO TO 300
60 IF (K .NE. 6) GO TO 70
STM=1.99244*H*1.54452*WW*.28158*W*WW*.02743
GO TO 300
70 IF (K .NE. 7) GO TO 80
STM=1.99124*H*1.54018*WW*.24706*W*WW*.02616
GO TO 300
80 IF (K .NE. 8) GO TO 90
STM=1.99038*H*1.53523*WW*.21676*W*WW*.02449
GO TO 300
90 IF (K .NE. 9) GO TO 100
STM=1.98978*H*1.52975*WW*.19029*W*WW*.02265
GO TO 300
100 IF (K .NE. 10) GO TO 110
STM=1.98939*H*1.52385*WW*.16723*W*WW*.02078
GO TO 300
110 IF (K .NE. 11) GO TO 120
STM=1.98915*H*1.51768*WW*.14716*W*WW*.01895
120  GO TO 300
130  IF (K .NE. 12) GO TO 130
     STM=1.98904+W*1.51133+WW*.1297-W*WW*.01721
     GO TO 300
140  IF (K .NE. 13) GO TO 140
     STM=1.989+W*1.50492+WW*.11449-W*WW*.01559
     GO TO 300
150  IF (K .NE. 14) GO TO 150
     STM=1.9892+W*1.49854+WW*.10123-W*WW*.0141
     GO TO 300
160  IF (K .NE. 15) GO TO 160
     STM=1.98906+W*1.49224+WW*.08964-W*WW*.01273
     GO TO 300
170  IF (K .NE. 16) GO TO 170
     STM=1.98912+W*1.48609+WW*.07949-W*WW*.01149
     GO TO 300
180  IF (K .NE. 17) GO TO 180
     STM=1.98917+W*1.48013+WW*.07057-W*WW*.01036
     GO TO 300
190  IF (K .NE. 18) GO TO 190
     STM=1.98921+W*1.47438+WW*.06273-W*WW*.00933
     GO TO 300
200  IF (K .NE. 19) GO TO 200
     STM=1.98924+W*1.46887+WW*.0558-W*WW*.00864
     GO TO 300
210  IF (K .NE. 20) GO TO 210
     STM=1.98928+W*1.46361+WW*.04966-W*WW*.00755
     GO TO 300
220  IF (K .NE. 21) GO TO 220
     STM=1.98922+W*1.45859+WW*.04322-W*WW*.00679
     GO TO 300
230  IF (K .NE. 22) GO TO 230
     STM=1.98918+W*1.45383+WW*.03936-W*WW*.00609
     GO TO 300
240  IF (K .NE. 23) GO TO 240
     STM=1.98912+W*1.44931+WW*.03502-W*WW*.00546
     GO TO 300
250  IF (K .NE. 24) GO TO 250
     STM=1.98905+W*1.44504+WW*.03114-W*WW*.00489
260  RETURN
END
C NORMALIZE DENSITY OF STATES

SUBROUTINE SMAX(A,1,IS1,IS2,K)
  REAL A(2,K),S1(2,K)
  S1=0.
  S2=0.
  DO 10 I=1,K
  IF (S1 .GE. A(I,1)) GO TO 20
  S1=A(I,1)
  IS1=I
  20 IF (S2 .GE. A(2,1)) GO TO 10
  S2=A(2,1)
  IS2=I
  10 CONTINUE
  X=X/S2
  Y=2/S2
  Z=2/S2
  DO 50 J=1,K
  A(I,J)=X*A(I,J)
  B(I,J)=Y*A(I,J)
  C(I,J)=Z*A(I,J)
  50 CONTINUE
  RETURN
END

C SMOOTH DATA

SUBROUTINE SMOOTH(A,1,K)
  REAL A(2,K)
  Y=A(I,J)
  Z=A(I,J)
  DO 10 J=3,K
  X=Y
  Y=Z
  Z=A(I,J)
  A(I,J-1)=.25*X+.54*Y+.25*Z
  10 CONTINUE
  RETURN
END
C PROBABILITY OF R

FUNCTION PR (X)
COMMON /FBK/ CR
T4=CR**X**3
FAC=1.0/(12.0*CR)**(1.0/3.0)*EXP(-2.0/3.0)
IF (TM<GT.50.) GO TO 10
PR=CR*3.*X**2*EXP(-TM)
PR=PR+FAC
GO TO 20
10 PR=0.
20 RETURN
END

C FIND BETA AND EF FOR GIVEN CONCENTRATION AND TEMPERATURE
SUBROUTINE BCT (XCS,TS,BETA,EF,IR)
REAL PFA (15),EF(5),R3(5)
COMMON /MBK/ RHC,RKE,KE,ED,EB,RNO,B0,PI
COMMON /FBK/ CR,AKT,CC,1
COMMON /RTBK/ XC,11
XC=XCS
T=TS
TT=T
A10=ALOG (10.)
C=10.*X*C
RK1=CB617*T/ED
RHC=RMIN*RHC*SQR((RME+T)**3
CC=C/RHC
CB=C*EB**3
CR=CB**4.*PI/3.
IF (TT>GT.60.) .IR. (XC<1.17.5)) GO TO 11
CALL FNRT (R3,IR)
GO TO 12
11 IR=1
R3(1)=RNDT(1-20.,5.)
12 DO 30 1=1,IR
EF(1)=R3(1)*A10*RK1
XF=10.***R3(11)
BETA(1)=SQR((BD+RHU+RHC+SQR(RME)**3*SQR(7.)*SMF'(XF))/RKE)*RD
30 CONTINUE
RETURN
END
BIBLIOGRAPHY


