THEORY OF AN ELECTRIC -CURRENT-FLOW INDUCED POLARIZATION EFFECT ON THE OPTICAL ABSORPTION OF A SEMICONDUCTOR

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ABSTRACT

THEORY OF AN ELECTRIC-CURRENT-FLOW INDUCED POLARIZATION EFFECT ON THE OPTICAL ABSORPTION OF A SEMICONDUCTOR

By Carl A. Baumgardner

A calculation is made of the direct optical absorption in a current-carrying semiconductor. It is assumed that the only effect of the d.c. electric field which produces the current, is to shift the distribution of carriers in $\underline{k}$ space. It is found that the absorption depends on the relative orientations of the electric field and the polarization vector of the light. This polarization effect is found to be proportional to the square of the carrier drift. A physical picture of the effect is presented. Curves of the effect versus photon energy are calculated for both fundamental and inter-valence-band absorption in indium antimonide, for both the intrinsic and extrinsic semiconductor, and for various field strengths and temperatures. The results are analyzed and found to be consistent with the physical picture of the effect. Suggestions are made for using the effect to investigate the distribution functions and wave functions of a semiconductor and a comparison is made with a similar effect measured in p-type germanium.

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I. INTRODUCTION

If a large external electric field is applied to a semiconductor in which there are free carriers, the most immediate result is a change in the energy distribution of those carriers. Many physical properties of semiconductors depend on the energy distribution of the carriers and it is to be expected that these properties will change with the electric field. Since the 1930's many such changes have been observed and studied; for example changes in the mobility and the Hall effect. New effects, such as negative resistance and anisotropies in the conductivity, have also been found to be associated with carrier streaming. It is evident that an understanding of the energy distribution of the carriers is fundamental to an understanding of these changes of physical properties which have come to be known as "hot-electron effects". The fact that our present-day knowledge of the distribution function as a function of the electric field is to a large extent only qualitative, is reflected in the large number of hot-electron effects for which there is not yet a good quantitative explanation.[1] The purpose of this paper is to extend the theoretical understanding of some recent experiments aimed at obtaining quantitative information about the distribution function under current flow conditions, and to propose some new experiments with the same objective.

Much of the earliest work on the effects of large electric fields on solids was directed toward understanding the energy distribution function.[2,3,4] Only recently, however have there been any successes in describing the distribution function quantitatively.[5,6] The most notable of these has been the work of Pinson and Bray[7] on the experimental determination of the distribution function in p-type germanium by means of "free-electron" absorption experiments. The facts that a unique correlation between the absorption frequency and the electronic energy of the absorbing state is possible, and that the amount of absorption at this frequency is a function of the number of carriers available to absorb the light, allowed the number of carriers as a function of the energy to be roughly determined.

It was noted by Pinson and Bray at that time,[8] as well as by others working independently,[9] that the absorption was dependent on the direction of polarization of the light relative to the electric field, and that this effect yields some additional details concerning the angular dependence of the hot-carrier distribution function. The complexity of the wave functions for p-type germanium prevented a complete quantitative analysis and thus impeded the theoretical explanation of the effect and the description of the distribution function. In this paper we predict a similar polarization effect for indium antimonide, and using the relatively simple wave functions given by Kane[10] for this semiconductor, we analyze the effect in detail. Consideration of the results yields a clear physical picture of the causes of the effect and shows that measurements of the effect not only can be a tool for understanding the distribution function, but also can yield information about the wave functions of the semiconductor.

In Chapter II of this paper the optical absorption coefficient is developed in a form particularly suited to our problem. In Chapter III the polarization effect is calculated in the approximation that the electronic wave vector, $\underline{k}$, is small. A physical explanation of the effect is given in Chapter IV. The restriction to small wave-vectors is removed in Chapter V and theoretical curves of the polarization effect versus photon energy for various distribution functions, temperatures and electric field strengths are computed; a discussion of the results is presented in Chapter VI.

II. THE ABSORPTION COEFFICIENT

The amount of light of a certain frequency, ω, absorbed by a crystal upon which it is incident, is described by the absorption coefficient,[11] defined by

$$\alpha(\omega) = \frac{\text{power absorbed per unit volume}}{\text{incident flux}} . \tag{2.1}$$

The power absorbed per unit volume is

$$\hbar\omega r_{ind} \tag{2.2}$$

where $\hbar$ is Planck's constant divided by 2π. r_{ind} is the net rate of transitions induced in the crystal by the light, per unit volume, per unit time, and is a function of the frequency. The incident flux is the magnitude of the time averaged Poynting vector,

$$\underline{S} = \frac{c}{4\pi} \overline{\underline{E}_L \times \underline{H}} . \tag{2.3}$$

$\underline{E}_L$ and $\underline{H}$ are the electric and magnetic field strengths of the incident light.

In Chapters III, IV, and V we shall be interested in calculating the absorption due to direct electron transitions between energy bands in a semiconductor (see figure 1). These can either be transitions between two valence bands (dotted lines), or between a valence band and the conduction band (solid lines). The former is sometimes called free-electron absorption, because it lies in the same frequency range

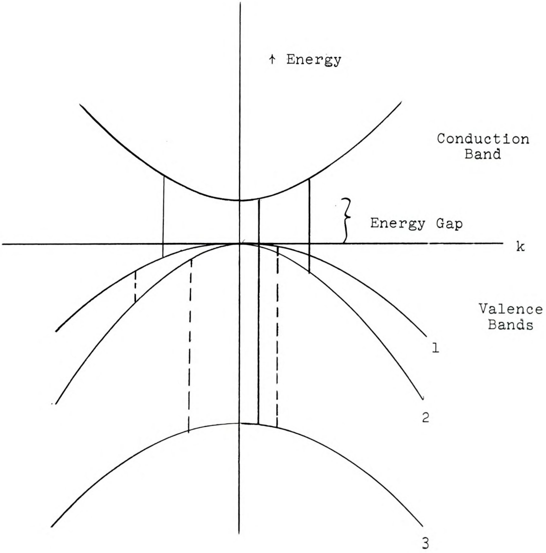


Fig. 1. Direct optical transitions

as true free-electron absorption, to distinguish it from the latter which is called fundamental absorption. in this paper we call them inter-valence band absorption and fundamental absorption, respectively.

The electric field of the light causing the transitions (not to be confused with the d.c. electric field, to be introduced later to modulate the absorption), can be described by a vector potential,

$$\underline{A}(\underline{r},t) = \underline{A}_0 \exp[i(\underline{s}\cdot\underline{r}-\omega t)] + \underline{A}_0^* \exp[-i(\underline{s}\cdot\underline{r}-\omega t], \qquad (2.4)$$

where $\underline{A}_0 = |\underline{A}_0|\exp(i\delta)\hat{a}_0$ is complex, $\hat{a}_0$ is a unit vector in the direction of $\underline{A}_0$, $\underline{s}$ is the wave vector and ω the frequency of the electromagnetic wave. Our first step in calculating the rate of induced transitions will be to find the interaction energy between this field and the electrons in the bands.

The interaction energy, H', is found from the classical Hamiltonian, H, for a particle of charge e and mass m in an electromagnetic field[12]:

$$H = \frac{1}{2m}\left(\underline{p} - \frac{e}{c}\underline{A}\right)^2 + e\Phi. \qquad (2.5)$$

$\underline{p}$ is the momentum, c the speed of light in a vacuum and Φ is the scalar potential of the electric field.

Multiplying out the squared term in Eq.(2.5), and using the relation

$$f(\underline{r})p_x - p_x f(\underline{r}) = i\hbar \frac{\partial}{\partial x} f(\underline{r}), \qquad (2.6)$$

which is true for any function that can be expressed in a power series in x, y, and z, we have

$$H = \frac{p^2}{2m} - \frac{e}{mc} \underline{A} \cdot \underline{p} + \frac{ie\hbar}{2mc} \underline{\nabla} \cdot \underline{A} + \frac{e^2}{2mc^2} A^2 + e\Phi. \tag{2.7}$$

Here $\underline{\nabla} = \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z}$

where $\hat{i}$, $\hat{j}$, $\hat{k}$, are unit vectors in the x,y,and z directions. We choose the transverse (Coulomb) gauge, so that

$$\underline{\nabla} \cdot \underline{A} = 0$$

$$\Phi = 0 \quad .$$

We also drop the term in A^2 as much smaller than the remaining terms. Adding to Eq. (2.7) the potential $V(\underline{r})$ of the electron in the periodic lattice and substituting $\underline{p} = -i \hbar \underline{\nabla}$, we arrive at the Hamiltonian for an electron in a periodic lattice interacting with an electric field. To first order

$$H = H_0 + H' \tag{2.9}$$

with

$$H_0 = \frac{-\hbar^2}{2m} \nabla^2 + V(\underline{r}), \tag{2.10}$$

and

$$H' = \frac{-e}{mc} \underline{A} \cdot \underline{p} \quad . \tag{2.11}$$

H_0 is the unperturbed Hamiltonian leading to the unperturbed band structure of the semiconductor, and H' is the interaction energy we have been seeking.

Using time dependent perturbation theory we can calculate[13] the probability that an electron in the valence-band state ϕ_v at time t=0 will be induced by the perturbation H' to change to the state ϕ_c in a higher band (perhaps but not necessarily the conduction band) at the later time t. This transition probability is given by

$$T^{o}_{cv}(t,\omega) = |<\phi_c|H_T'|\phi_v>|^2 \times S(E) \tag{2.12}$$

where

$$S(E) = \frac{4\,\mathrm{Sin}^2[(E_c(k) - E_v(k) - \hbar\omega)t/2\hbar]}{[E_c(k) - E_v(k) - \hbar\omega]^2}, \tag{2.12b}$$

<> indicates the quantum mechanical expectation, and

$$H_T' = -\frac{e}{mc}\exp(i\underline{s}\cdot\underline{r})\underline{A}_o\cdot\underline{p}. \tag{2.13}$$

$E_c(k_c)$ and $E_v(k_v)$ are the electron energies in states ϕ_c and ϕ_v respectively, and are functions of $\underline{k}$ the wave vector of the electron.

T^{o}_{cv} is not the total transition probability. We must multiply it by an occupation factor (distribution function), $f(E_v)$, which is the probability that the state ϕ_v is occupied, and also by the occupation factor $[1 - f(E_c)]$ which is the probability that the state ϕ_c is not occupied. Thus the total probability of a transition from state ϕ_v to state ϕ_c is

$$T_{cv} = |<\phi_c|H_T'|\phi_v>|^2 S(E)\{f(E_v)[1 - f(E_c)]\} \tag{2.14}$$

The probability that an electron in state ϕ_c at time t = 0 will be induced by H' to change to the state ϕ_v at time t, can also be found by time-dependent perturbation theory. It is

$$T^{o}_{vc} = |\langle\phi_v|H_T''|\phi_c\rangle|^2 \times S(E), \qquad (2.15)$$

where

$$H_T'' = \frac{-e}{mc} \exp\,(-i\underline{s}\cdot\underline{r})A_o^{*}\cdot\underline{p}. \qquad (2.16)$$

It can be shown[14]

$$|\langle\phi_c|H_T'|\phi_v\rangle|^2 = |\langle\phi_v|H_T''|\phi_c\rangle|^2 \qquad (2.17)$$

therefore

$$T^{o}_{vc} = T^{o}_{cv} \qquad (2.18)$$

The occupation factor for T_{vc} is $f(E_c)[1 - f(E_v)]$. Therefore the net transition probability (the probability for transitions upward minus the probability for transitions downward) is

$$T^{N}_{cv} = T_{cv} - T_{vc} = |\langle\phi_c|H_T'|\phi_v\rangle|^2\ S(E)\ [f(E_v) - f(E_c)] \qquad (2.19)$$

The rate of transitions is found by summing the transition probabilities for all possible combinations of ϕ_c and ϕ_v and dividing by t. In the most general case the summation is performed by multiplying by the density of states per unit volume, $\frac{1}{(2\pi)^3}$, and integrating over the two bands c and v. However conservation of momentum requires that the momentum of the electron in the initial state plus the momentum of the photon must equal the momentum of the electron in the final state; i.e.

$$\hbar\underline{k}_v + \hbar\underline{s} = \hbar\underline{k}_c. \qquad (2.20)$$

But $\underline{s}$ is so much smaller than $\underline{k}_v$ or $\underline{k}_c$ that essentially

$$\underline{k}_v = \underline{k}_c.$$

This establishes a one-to-one correspondence between the two states ϕ_v and ϕ_c which allows all possible combinations of ϕ_v and ϕ_c to be included simply by integrating once over all k space. Therefore

$$r_{ind} = \frac{1}{t}\int|<\phi_c|H_T'|\phi_v>|^2\ S(E)\ \times$$
$$\frac{k^2}{(2\pi)^3}[f(E_v) - f(E_c)]\ \mathrm{Sin}\theta\ d\theta d\phi dk. \qquad (2.22)$$

To find the magnitude of $\overline{S}$ we use

$$\underline{E}_L = -\frac{1}{c}\frac{\partial A}{\partial t} = -\frac{2\omega}{c}|A_o|\ \mathrm{Sin}\ (\underline{s}\cdot\underline{r} - \omega t + \delta)\hat{a}_o,$$

$$H = \underline{\nabla} \times A = -2\underline{s} \times \hat{a}_o|A_o|\ \sin\ (\underline{s}\cdot\underline{r} - \omega t + \delta), \qquad (2.23)$$

$$\overline{\sin^2(\underline{s}\cdot\underline{r} - \omega t + \delta)} = \frac{1}{2},$$

and

$$\frac{kc}{\omega} = n = \text{index of refraction}. \qquad (2.24)$$

Then using Eq. (2.3) we have,

$$|S| = \frac{n\omega^2}{2\pi c}|A_o|^2. \qquad (2.25)$$

From Eqs. (2.25), (2.22) and (2.1) we arrive at the absorption coefficient:

$$\alpha(\omega) = \frac{e^2\hbar}{4\pi^2 nm^2 c\omega t} \int |\langle\phi_c|\hat{a}_o\cdot\underline{p}|\phi_v\rangle|^2 \, S(E)$$

(2.26)

$$[f(E_v) - f(E_c)]\underline{k}^2 \sin\theta \, d\theta d\phi.$$

We have used the fact that s is essentially zero to drop the exp $(i\underline{s}\cdot\underline{r})$ in the matrix element.

The integral over k in Eq. (2.26) can be done immediately even though we do not have explicit expressions for the k- dependence of the energy or distribution function. This is possible because in the limit of large time, t, we have for S(E) (Eq.(2.12b)):

$$\lim_{t\to\infty} \frac{4 \sin^2[\{E_c(k)-E_v(k)-\hbar\omega\}t/2\hbar]}{[E_c(k)-E_v(k)-\hbar\omega]^2} = \frac{2\pi t}{\hbar} \delta[E_c(k)-E_v(k)-\hbar\omega]$$

(2.27)

Taking this limit makes sense physically if the light has been turned on for a time long compared to the inverse of its frequency, which is generally true experimentally. Using

$$\delta[f(x)] = \frac{1}{\left|\frac{df}{dx}\right|} \delta(x - x_o) \qquad (2.28)$$

Eq. (2.26) then becomes

$$\alpha(\omega) = \frac{e^2 k^2}{2\pi m^2 c n\omega} \int \frac{|\langle\phi_c|\hat{a}_o\cdot\underline{p}|\phi_v\rangle|^2 \sin\theta \, [f(E_v) - f(E_c)] d\theta d\phi}{\left|\frac{d(E_c - E_v)}{dk}\right|},$$

(2.29)

where k is now determined by

$$E_c(k) - E_v(k) - \hbar\omega = 0 \tag{2.30}$$

If there are more than two bands involved in the transitions we must sum Eq. (2.29) over all possible combinations of bands. The total absorption coefficient is then

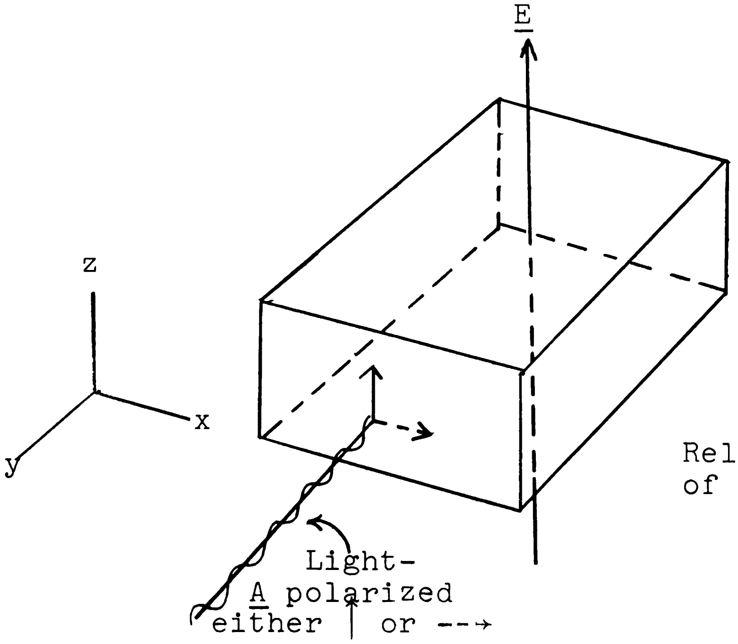
$$\alpha(\omega) = \sum_c \sum_v \frac{e^2k^2}{2\pi m^2 cn\omega} \int \frac{|\langle\phi_c|\hat{a}_o \cdot \underline{p}|\phi_v\rangle|^2[f(E_v)-f(E_c)] \sin\theta d\theta d\phi}{\left|\frac{d\ (E_c - E_v)}{dk}\right|}. \tag{2.31}$$

To proceed any further in a calculation of the absorption coefficient we need explicit expressions for the matrix element, the energies and the distribution functions.

III. THE POLARIZATION EFFECT IN THE LIMIT OF SMALL CARRIER WAVE-VECTOR

In this chapter we calculate the absorption coefficient for intrinsic indium antimonide with a d.c. electric field, $\underline{E}$ (which shall always appear with a vector sign to distinguish it from the energy), applied perpendicular to the direction of propagation of the light (See Figure 2). We take the electric field to be in the z-direction and consider two cases. In one case the vector potential, $\underline{A}$, is directed parallel to $\underline{E}$, and in the other $\underline{A}$ is directed perpendicular to $\underline{E}$. The difference in the absorption for these two cases is the polarization effect. We consider in this chapter only the absorption due to transitions between a valence band and the conduction band; i.e. the fundamental absorption, and this is calculated in the approximation of small k (electron wave-vector magnitude).

We assume that the d.c. electric field does not change the band structure of the crystal. This assumption is thought to be valid because many collisions take place during the characteristic time of a polarization effect experiment, which washes out changes that would otherwise require consideration.[15] We have chosen indium antimonide as the model semiconductor for our calculation because of its high mobility, which permits a large shift in its



Relative orientations of E and A.

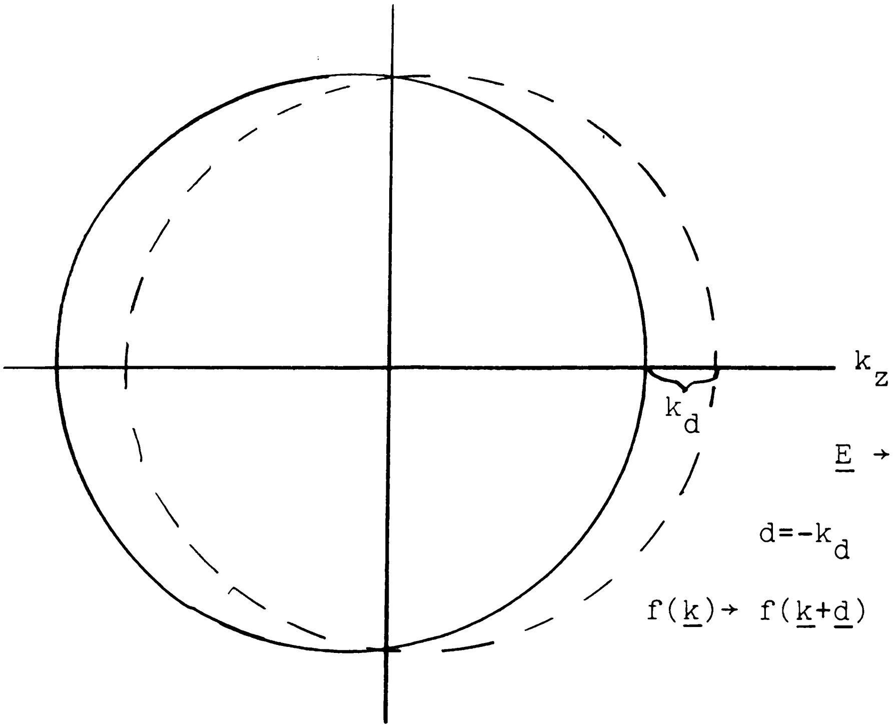


Fig. 2. Shift of electrons in k-space under the influence of an electric field.

distribution function with relatively small electric fields, and because accurate, relatively simple analytic expressions for its wave functions are available.

1. The Band Structure

The wave functions and energies for indium antimonide have been calculated by Kane.[10] He added to the classical Hamiltonian Eq. (2.9), several spin dependent terms and applied the resulting Schroedinger equation to the Bloch function, exp $(i\underline{k}\cdot\underline{r})u_K(\underline{r})$, to arrive at the Schroedinger equation for the cell-periodic function $u_K(\underline{r})$, which we write as

$$\left[\frac{\underline{p}^2}{2m} + V(\underline{r}) + \frac{\hbar}{m}\underline{k}\cdot\underline{p} + \frac{\hbar k^2}{2m} + S_1\right]u_K(\underline{r}) = E_K u_K(\underline{r}). \quad (3.1)$$

The first four terms result from the classical Hamiltonian and S_1 is a spin-dependent term added by Kane. We have dropped a second spin-dependent term because Kane found it very small.

The solutions of Eq. (3.1) are found in terms of the solutions of

$$\left[\frac{\underline{p}^2}{2m} + V\right]U_i = E_i U_i \quad (3.2)$$

These solutions are known from group theory to be S↑ and S↓ for the conduction band, and X↑, X↓, Y↑, Y↓, Z↑, and Z↓ for the valence bands. S signifies a function with the symmetry properties of an atomic s orbital under the operations of the tetrahedral group, and X, Y, and Z signify wave functions with symmetry properties of the x, y, z atomic p-functions. The s functions have energy E_s and the p functions all have energy E_p.

For $\underline{k}$ in the z direction, Kane solved the Hamiltonian matrix corresponding to Eq. (3.1) for its eigenvalues which he found to be given by the equations

$$E' = 0 \tag{3.3}$$

$$E'(E' - E_G)(E' + \Delta) - k^2\underline{P}^2(E' + 2\Delta/3) = 0. \tag{3.4}$$

Here $E_G = E_s$, $\Delta = -3E_p$,

$$E' = E_K - (\hbar^2/2m)k^2, \tag{3.5}$$

$$\underline{P} = -\frac{i\hbar}{m}\langle s|p_z|z\rangle, \tag{3.6}$$

and m is the free electron mass.

E_G is the energy gap and Δ is the energy separation of the "split-off band"; i.e. a valence band which is lower in energy than the other two bands which are degenerate at $\underline{k} = 0$. Both parameters can be evaluated experimentally.

If k^2 is very small Eq. (3.4) is approximately equal to

$$E'(E' - E_G)(E' + \Delta) = 0, \tag{3.7}$$

which has the solutions

$$E' \simeq 0,\ E' \simeq E_G,\ E' \simeq -\Delta. \tag{3.8}$$

We can find an approximate solution of Eq. (3.4) corresponding to each of these three values by writing it in the form

$$(E' - E_o) = f(E'), \tag{3.9}$$

where E_o is one of the values Eq. (3.8).

Then substituting this same E_o for the E's on the right we have

$$E_c = E_G + \frac{\hbar^2 k^2}{2m} + \frac{P^2 k^2}{3}\left(\frac{2}{E_G} + \frac{1}{[E_G + \Delta]}\right) = E_G + \frac{\hbar^2 k^2}{2m_c} \tag{3.10}$$

$$E_2 = \frac{\hbar^2 k^2}{2m} - 2\frac{P^2 k^2}{3E_G} = -\frac{\hbar^2 k^2}{2m_2} \tag{3.11}$$

$$E_3 = -\Delta + \frac{\hbar^2 k^2}{2m} - \frac{P^2 k^2}{3(E_G + \Delta)} = -\Delta - \frac{\hbar^2 k^2}{2m_3} \tag{3.12}$$

The highest valence band is the solution of Eq. (3.3), which is

$$E_1 = \frac{\hbar^2 k^2}{2m}. \tag{3.13}$$

This is inaccurate, as explained by Kane, so we use instead

$$E_1 = -\frac{\hbar^2 k^2}{2m_1}, \tag{3.14}$$

where m_1 is given experimentally. E_c is the conduction band, E_1 is the heavy mass band, E_2 is the light mass band and E_3 is the split-off band.

The wave functions that result from the diangonalization of the Hamiltonian corresponding to Eq. (3.1) are:

$$\begin{aligned} \phi_{i\alpha} &= a_i[iS\downarrow]' + b_i[(X - iY)\uparrow/\sqrt{2}]' + c_i[Z\downarrow]' \\ \phi_{i\beta} &= a_i[iS\uparrow]' + b_i[-(X + iY)\downarrow/\sqrt{2}]' + C_i[Z\uparrow] \end{aligned} \tag{3.15}$$

$$\begin{aligned} \phi_{1\alpha} &= [(X + iY)\uparrow]'/\sqrt{2} \\ \phi_{1\beta} &= [(X - iY)\downarrow]'/\sqrt{2} \end{aligned} \tag{3.16}$$

The index i takes on the values c, 2, 3 referring to the conduction band, the second valence band and the third valence band. The 1 refers to the first valence band. Wave functions with first subscript the same but different in the second subscript (α or β) are degenerate in energy but differ in spin. The primes in Eqs. (3.15) and (3.16) indicate that for directions of $\underline{k}$ other than the z-direction, X', Y', Z', S', $\uparrow'$ and $\downarrow'$ are obtained by the transformations:

$$\begin{bmatrix} \uparrow' \\ \\ \downarrow' \end{bmatrix} = \begin{bmatrix} \exp\,(-i\phi/2)\,\cos\,(\theta/2) & \exp\,(i\phi/2)\,\sin\,(\theta/2) \\ \\ -\exp\,(-i\phi/2)\,\sin\,(\theta/2) & \exp\,(i\phi/2)\,\cos\,(\theta/2) \end{bmatrix} \begin{bmatrix} \uparrow \\ \\ \downarrow \end{bmatrix} \tag{3.17}$$

$$\begin{bmatrix} X' \\ Y' \\ Z' \end{bmatrix} = \begin{bmatrix} \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} \tag{3.18}$$

$$S' = S \tag{3.19}$$

θ is the angle k makes with the z-axis and ϕ is the angle k makes with the x-axis.

The a_i, b_i, and c_i are real coefficients given by:

$$\begin{aligned} a_i &= kP(E_i' + 2\Delta/3)/N \\ b_i &= (\sqrt{2}\Delta/3)(E_i' - E_G)/N \qquad (3.20) \\ c_i &= (E_i' - E_G)(E_i' + 2\Delta/3)/N \end{aligned}$$

where $N = (a_i^2 + b_i^2 + c_i^2)^{1/2}$ and the E_i' are the solutions of Eq. (3.4). For small k Eqs. (3.20) become:

$$a_c = 1, \quad b_c = c_c = 0 \qquad (3.21)$$

$$a_2 = 0, \quad b_2 = (1/3)^{1/2}, \quad c_2 = (2/3)^{1/2}$$

$$a_3 = 0, \quad b_3 = (2/3)^{1/2}, \quad c_3 = -(1/3)^{1/2}$$

2. The Matrix Elements

Including spin differences, there are six valence bands and two conduction bands. Therefore in the summation over the conduction and valence bands in Eq. (2.31) we will have twelve terms. We must calculate the matrix element for each of these twelve terms and for each of the two directions of polarizations of the vector potential $\underline{A}$. Thus there are twenty-four matrix elements to be calculated. In the small $\underline{k}$ limit many of the coefficients of the wave functions, as given in Eq. (3.21), are zero. However we shall derive the matrix elements for the general case, where the coefficients are non-zero, since we shall need them in that form in a later chapter.

The following properties of the wave function will be useful in calculating the matrix elements:

a) In the absence of spin-dependent terms in the perturbing Hamiltonian

$$\begin{aligned}\langle\uparrow'|\downarrow'\rangle &= \langle[\exp(i\phi/2)\cos(\theta/2)\uparrow + \exp(-i\phi/2)\sin(\theta/2)\downarrow]| \\ &\quad |[-\exp(-i\phi/2)\sin(\theta/2)\uparrow + \exp(i\phi/2)\cos(\theta/2)\downarrow]\rangle \\ &= 0 \qquad (3.22)\end{aligned}$$

and likewise

$$\langle\downarrow'|\uparrow\rangle = 0;\ \langle\uparrow'|\uparrow'\rangle = 1;\ \langle\downarrow'|\downarrow'\rangle = 1. \qquad (3.23)$$

b) Electric dipole selection rules, group theory, and Eq. (3.6) yield:

$$\langle S|p_z|Z\rangle = \langle S|p_x|X\rangle = \frac{imP}{\hbar} \qquad (3.24)$$

$$\langle Z|p_z|S\rangle = \langle X|p_x|S\rangle = -\frac{imP}{\hbar} \qquad (3.25)$$

$$\langle S|p_i|J\rangle_{J\neq i} = 0;\ J = X,Y,Z;\ i = x,y,z \qquad (3.26)$$

$$\langle J|p_i|K\rangle = 0;\ i = x,y,z;\ J = X,Y,Z;\ K = X,Y,Z \qquad (3.27)$$

We now calculate, as an example, the matrix element $\langle\phi_{c\alpha}|\hat{a}_o\cdot\underline{p}|\phi_{2\beta}\rangle$ for $\underline{A}$, (i.e., $\hat{a}_o$) in the x-direction.

$$\hat{a}_o \cdot \underline{p} = \hat{i} \cdot \underline{p} = p_x .$$

$$<\phi_{c\alpha}|p_x|\phi_{2\beta}> = <a_c[-iS\downarrow{}'] + b_c[(X + iY)\uparrow/\sqrt{2}]' + c_c(Z\downarrow]'|p_x$$

$$|a_2[iS\uparrow]' + b_2[-(X+iY)\downarrow/\sqrt{2}]' + c_2[Z\downarrow]'>$$

[Using Eqs. (3.22) and (3.23)] $= <a_c[-iS]'|p_x|b_2[-(X + iY)/\sqrt{2}]'> +$

$$+ <b_c[(X + iY)/\sqrt{2}]'|p_x|a_2[iS]'>$$

[Using Eqs. (3.18) and (3.19)] $= <a_c[-iS]|p_x|b_2[-(\cos\phi \cos\theta X + \cos\phi \sin\phi Y -$

$$\sin\theta Z) - i(-\sin\phi X + \cos\phi Y)]> +$$

$$+ <b_c[(\cos\theta \cos\phi X + \cos\theta \sin\phi Y - \sin\theta Z) +$$

$$+ i(-\sin\phi X + \cos\phi Y)]|p_x|a_2[iS]>,$$

[Using Eqs. (3.26) and (3.27)] $= i\frac{a_c b_2}{\sqrt{2}}(\cos\theta \cos\phi - i \sin\phi)<S|p_x|X> +$

$$+ i\frac{b_c a_2}{\sqrt{2}}(\cos\theta \cos\phi - i \sin\phi)<X|p_x|S>,$$

[Using Eqs. (3.24) and (3.25)] $= mP/(\hbar\sqrt{2})(\cos\theta \cos\phi - i \sin\phi)(b_c a_2 - a_c b_2).$

The twenty-four matrix elements calculated in this way are listed in Table I. In this table $i = 2,3$, $D = mP/\hbar$, $G_{i+} = (a_c c_i + c_c a_i)$, and $G_{i-} = (a_c b_i - b_c a_i)$.

TABLE I.--The matrix elements between the conduction and valence bands in In Sb.

$\underline{A}$ in z-direction				
	$\phi_{i\alpha}$	$\phi_{i\beta}$	$\phi_{l\alpha}$	$\phi_{l\beta}$
$\phi_{c\alpha}$	$D\cos\theta G_i +$	$(\frac{D}{\sqrt{2}})\sin\theta G_i -$	0	$-(\frac{D}{\sqrt{2}})a_c\sin\theta$
$\phi_{c\beta}$	$-(\frac{D}{\sqrt{2}})\sin\theta G_i -$	$D\cos\theta G_i +$	$-(\frac{D}{\sqrt{2}})a_c\sin\theta$	0

$\underline{A}$ in x-direction				
	$\phi_{i\alpha}$	$\phi_{i\beta}$	$\phi_{l\alpha}$	$\phi_{l\beta}$
$\phi_{c\alpha}$	$D\sin\theta\cos\phi G_i +$	$-\frac{D}{\sqrt{2}}(\cos\theta\cos\phi -$ $\sin\phi)G_i -$	0	$\frac{Da_c}{\sqrt{2}}(\cos\theta\cos\phi +$ $i\sin\phi)$
$\phi_{c\beta}$	$\frac{D}{\sqrt{2}}(\cos\theta\cos\phi +$ $i\sin\phi)G_i -$	$D\sin\ \cos\phi G_i +$	$\frac{Da_c}{\sqrt{2}}(\cos\theta\cos\phi -$ $i\sin\phi)$	0

3. The Distribution Functions for Electrons and Holes

We assume that the effect of the electric field is to shift the distribution of carriers in k-space by the amount k_d. This is shown in Figure 2 for a Fermi-sphere.

For non-zero temperatures the sphere of course will not be sharply defined but will be "blurred" near the edge. At zero electric field, the carriers will have the distribution given by the dotted circle. When the electric field is applied in the positive z-direction the distribution shifts in the negative z-direction by the amount k_d. Thus carriers at $\underline{k}$ with a certain energy, $E(\underline{k})$ will have an occupation probability corresponding to $\underline{k} + \underline{d}$ of the unshifted distribution. d is a positive number which is equal to $-k_d$, the size of the shift in k due to the electric field. k_d has the same sign for the conduction and valence bands although in our problem the sign is not important since the polarization effect is independent of this sign.

For the small k calculation we take the distribution functions to be:

$$\exp \{[E_F - E_c(\underline{k} + \underline{d})]/KT\} \tag{3.29}$$

for the conduction band, and

$$1 - \exp \{[E_v(\underline{k} + \underline{d}) - E_F]/KT\} \tag{3.30}$$

for the valence bands. E_F is the Fermi energy, T is the temperature, and K is Boltzmann's constant. These are Fermi-Dirac distribution functions in the limit

$$|E - E_F| >> KT. \tag{3.31}$$

Eq. (3.31) is valid for intrinsic In Sb at all but very high temperatures, except near the conduction-band edge where it is good only up to about 300°K. Eqs. (3.29) and (3.30) are not necessarily the actual distribution functions for In Sb. More likely the experimental crystal will be an extrinsic semiconductor with some form of Maxwell-Boltzmann distribution function with the normalization depending on the concentration of impurities. However, these distribution functions do have the essential Boltzmann factor, and furthermore the simplicity of the intrinsic situation will make the physical interpretation of the theory clearer.

4. Calculation of the Polarization Effect

We now have explicit expressions for all the factors in Eq. (2.31). We calculate the absorption due to transitions between valence band one and the conduction band for the case when A is polarized in the x-direction, perpendicular to the d.c. electric field, as an example.

Substituting Eqs. (3.10) and (3.14) in Eqs. (3.29) and (3.30) we have:

$$f(E_c) = \exp\{[E_F-E_G-\frac{\hbar^2}{2m_c}(k_1^2+d_c^2+2k_1d_c \cos \theta)]/KT\} \quad (3.32)$$

$$f(E_v) = 1-\exp\{[\frac{-\hbar^2}{2m_1}(k_1^2+d_1^2+2k_1d_1 \cos \theta)-E_F]/KT\} \quad (3.33)$$

We have used

$$(\underline{k} + \underline{d})\cdot(\underline{k} + \underline{d}) = k^2 + d^2 + 2kd \cos \theta, \quad (3.34)$$

and we have written k with a subscript because k is different for transitions between different bands according to Eq. (2.30).

Substituting Eqs. (3.32), (3.33), (3.10) and (3.14) in (2.31) and summing over the four matrix elements involved (two of which are zero), we have:

$$\alpha_\perp^1(\omega) = \frac{3}{8\pi}\alpha_o^1\int(\cos^2\theta\cos^2\phi+\sin^2\phi)\sin\theta[1-A_{11}\exp(V_{11}\cos\theta)$$

$$-A_{c1} \exp(-V_{c1} \cos \theta)]d\theta d\phi,$$

where we have written

$$\alpha_o^1 = \frac{4e^2a_c^2P^2|k_1|}{3cn\omega\hbar^4\left|\frac{1}{m_c} + \frac{1}{m_1}\right|} \tag{3.36}$$

$$A_{11} = \exp\ \{[\frac{-\hbar^2}{2m_1}(k_1^2 + d_1^2) - E_F]/KT\} \tag{3.37}$$

$$A_{c1} = \exp\ \{[E_F - E_G - \frac{\hbar^2}{2m_c}(k_1^2 + d_c^2)/KT\} \tag{3.38}$$

$$V_{11} = -\frac{\hbar^2k_1d_1}{m_1KT} \tag{3.39}$$

$$V_{c1} = \frac{\hbar^2k_1d_c}{m_cKT}\ . \tag{3.40}$$

α_o^1 is the absorption in the limit T = 0, E = 0, for transactions between valence band 1 and the conduction band.

The integral over ϕ gives a factor of π. The integral over θ can be simplified with the change of variable $\cos\theta = x$ which implies $-\sin\theta d\theta = dx$. Eq. (3.35) then becomes:

$$\alpha_\perp^1 = \frac{3}{8}\alpha_o^1 \int_{-1}^{1} (x^2 + 1)(1 - A_{11}e^{V_{11}x} - A_{c1}e^{-V_{c1}x})dx, \tag{3.41}$$

which integrates to

$$\alpha^1_\perp = \tfrac{3}{4}\alpha^1_o\{\tfrac{4}{3} - A_{11}[\frac{(e^{V_{11}}-e^{-V_{11}})}{V_{11}} - \frac{(e^{V_{11}}+e^{-V_{11}})}{V_{11}^2} + \frac{(e^{V_{11}}-e^{-V_{11}})}{V_{11}^3}]$$

$$-A_{c1}[\frac{(e^{V_{c1}}-e^{-V_{c1}})}{V_{c1}} - \frac{(e^{V_{c1}}+e^{-V_{c1}})}{V_{c1}^2} + \frac{(e^{V_{c1}}-e^{-V_{c1}})}{V_{c1}^3}]\} \tag{3.42}$$

On expanding the exponentials for

$$|\ V_{ij}\ | << 1 \tag{3.43}$$

we find

$$\alpha^1_\perp = \alpha^1_o\{1-A_{c1}-A_{11} - \frac{A_{c1}V^2_{c1}}{4} \quad \frac{A_{11}V^2_{11}}{4}\ \}$$

Eq. (3.43) is valid if

$$\hbar^2\frac{k_j d_i}{m_i} << KT \tag{3.44}$$

Since we have already assumed k is small this is good if d_i is small: i.e. the drift velocity in band i must be much less than the thermal velocity, which is true in InSb for fields of 100v/cm or less.

Similarily we find:

$$\begin{aligned}
\alpha^1_{||} &= \alpha^1_o[1-A_{c1}-A_{11}] \\
\alpha^2_\perp &= \alpha^2_o[1-A_{c2}-A_{22}-\tfrac{1}{12}(A_{c2}V^2_{c2} + A_{22}V^2_{22})] \\
\alpha^2_{||} &= \alpha^2_o[1-A_{c2}-A_{22}-\tfrac{1}{3}(A_{c2}V^2_{c2} + A_{22}V^2_{22})] \\
\alpha^3_{||} &= \alpha^3_\perp = \alpha^3_o[1-A_{c3}-A_{33}-\tfrac{1}{6}(A_{c3}V^2_{c3} + A_{33}V^2_{33})]
\end{aligned} \tag{3.45}$$

where α_i^o, A_{ci}, A_{ii}, V_{ci}, V_{ii}, $i = 2, 3$ are given by Eqs. (3.36) through (3.40) with obvious changes in the subscripts. $||$ and $\perp$ indicate the relative orientations of $\underline{E}$ and $\underline{A}$.

The polarization effect is given by

$$\alpha_p^i = \alpha_{||}^i - \alpha_{\perp}^i \text{ , } i = 1,2,3.$$

Thus we have

$$\alpha_p^1 = \frac{\alpha_o^1}{4} [A_{c1}V_{c1}^2 + A_{11}V_{11}^2] \qquad (3.46)$$

$$\alpha_p^2 = -\frac{\alpha_o^1}{4} [A_{c2}V_{c2}^2 + A_{22}V_{22}^2] \qquad (3.47)$$

$$\alpha_p^3 = 0 \qquad (3.48)$$

The polarization effect (Eqs. (3.46) through (3.48) is roughly proportional to $\underline{E}^2$ through the variables V_{ij}^2. The factors in the A's which are proportional to $\underline{E}$ (d_i^2 in Eq. (3.37) for example) are not important, since d is very small, which makes exp (-d) nearly 1 and slowly varying. The effect goes to zero with $\underline{E}$ as expected, however the difference in signs of the first two equations and the zero result for the last is noteworthy. This last result becomes even more interesting when the integrals analogous to Eq. (3.35) are written out for these transitions. One finds the effect is identically zero no matter what distribution function is used. This points to the wave functions as the cause of the peculiarites and as we shall see in the next chapter, this inference is correct.

IV. THE PHYSICAL EXPLANATION OF THE POLARIZATION EFFECT

In Chapter III we suggested connections between certain features of the wave functions and certain peculiarities of the polarization effect. To clarify these connections we investigate the matrix elements for the different polarizations and different directions of electronic motion given by $\underline{k}$, for an idealized set of wave functions.

Consider transitions between a conduction band with a purely S-like wave function and a valence band with a Z- like wave function, when $\underline{k}$ is in the z-direction. For $\underline{A}$ also polarized in the z-direction, the matrix element is

$$\langle S|p_z|Z\rangle = M \quad . \tag{4.1}$$

If we now take $\underline{k}$ in the x-direction, S→S and Z→X by transformations (3.18) and (3.19). Thus the matrix element is

$$\langle S|p_z|X\rangle = 0. \tag{4.2}$$

Now take $\underline{A}$ to be polarized in the x-direction. For $\underline{k}$ in the z-direction the matrix element is

$$\langle S|p_x|Z\rangle = 0, \tag{4.3}$$

and for $\underline{k}$ in the x-direction it is

$$\langle S|p_x|X\rangle = M. \tag{4.4}$$

Next we calculate the absorption associated with the two directions of $\underline{k}$. (Picture two electrons doing the absorbing, one moving in the z-direction and one moving in the x-direction with the same speed; i.e. the same magnitude of $\underline{k}$.) Because the energy is a spherically symmetric function of $\underline{k}$ we have

$$\alpha_z = [|M|^2 + 0]\, D = |M|^2 D, \tag{4.5}$$

$$\alpha_x = [0 + |M|^2]\, D = |M|^2 D, \tag{4.6}$$

where α_z and α_x are the absorptions for the light polarized in the z- and x-directions respectively and D is some constant which depends on the magnitude of $\underline{k}$. We see the sum total of α_z and α_x is the same for these directions. We call the z and x directions corresponding directions because what one contributes to α_x the other contributes to α_z, and vice versa.

When we consider the absorption due to electrons moving in other directions, we find, because of the spherical symmetry of the transformation equations and the energy, that for each direction β_z there is a corresponding direction β_x that gives the same contribution to α_x as β_z gives to α_z and vice versa. This is a one-to- one and single valued correspondence. When we integrate over all angles as prescribed by Eq. (2.31), we find that $\alpha_z = \alpha_x$ just as in Eqs. (4.5) and (4.6).

If we now insert in the absorption expression an angularly dependent distribution factor, -exp(Cosθ), like the one due to an electric field in the z-direction, then, for k also in the z-direction

$$\alpha_z = \langle S|\, p_z \,|Z\rangle\; D\;\; [-\exp(1)] = -\; |M|^2\; De$$

$$\alpha_x = \langle S\; |p_x|\; Z\rangle\; D\;\; [-\exp(1)] = 0.$$

For k in the x-direction

$$\alpha_z = \langle S\; |p_z|\; X\rangle D\; [-\exp(0)] = 0$$

$$\alpha_x = \langle S\; |p_x|\; Z\rangle D\; [\; -\exp(0)] = -|M|^2\; D$$

Adding up the total absorption for the two directions of k we have

$$\alpha_z = [-|M|^2\; De+0] = -|M|^2\; De,$$

$$\alpha_x = [\; 0 - |M|^2\; D\;] = -\; |M|^2 D,$$

and therefore

$$\alpha_z - \alpha_x = \alpha|| - \alpha\perp \;= -\; |M|^2 D\; (e-1)$$

Thus there is a polarization effect because the absorption contribution from each of the corresponding directions x and z is multiplied by a different occupation factor. Likewise when we integrate over all angles there will be a polarization effect for the same reason. The field acts to lower the absorption because of the negative sign of the distribution factor.

We can now understand the reason for the sign difference between Eqs. (3.46) and (3.47). The wave functions for small k given by Eqs. (3.15) and (3.16) with coefficients (3.21) show that for k in the z-direction valence band number one has no Z component. Thus it contributes little or nothing to $\alpha_z \equiv \alpha_{||}$ when the distribution factor is large. At the same time it contributes most to $\alpha_x \equiv \alpha_{\perp}$ when the distribution factor is large. Thus the action of the distribution factor is larger for $\alpha_{\perp}$ than $\alpha_{||}$, and because the sign of this action is negative, the resulting polarization effect is positive.

Valence band two, however, has a much larger contribution from the Z-like wave than the X-like wave. Thus it will tend to contribute more to $\alpha_{||}$ and less to $\alpha_{\perp}$ when the distribution factor is large. Therefore the action on $\alpha_{||}$ is larger than the action on $\alpha_{\perp}$ and the sign of the distribution factor makes Eq. (3.47) negative.

The cause of the zero result for the third valence band is also to be found in the coefficients (3.21.). Because the relative probability of an electron, in this band, being in the state X, Y, or Z is given by the square of the respective coefficients of these functions, we see from Eqs. (3.21) and (3.15) that the probability of an electron's being in X + i Y is twice the probability of its being in Z. Dividing the probability of being in X and Y equally between the two, we find the probabilities of being in X,Y, or Z are all equal.

This is true for all directions of k because of the spherical symmetry of the transformations (3.18). Thus for any given direction, $\alpha \|$ = $\alpha \perp$; i.e. the corresponding directions are the same, and the distribution function can make no difference.

The description of the polarization effect for small k can be made in the simple terms used above because the conduction band is completely S-like in this limit. Away from k = 0 the conduction band rapidly becomes a mixture of all four orbitals, and the valence bands take on some S-like character and depart from the simple combinations of X, Y, and Z orbitals that made the above analysis so unambiguous. No matter how complicated the admixtures become, however, an analysis similar to that above can be carried out with the additional requirement that transitions proceeding downwards from the conduction band to a valence band (or from a higher valence band to a lower valence band), are negative additions to the absorption.

V. THE POLARIZATION EFFECT FOR ARBITRARY WAVE VECTOR

The approximate determination of the polarization effect given in Chapter III cannot be used to plot a curve of absorption versus frequency for a comparison with experiment because the wave functions for small $\underline{k}$ rapidly lose accuracy as we move just a small interval in frequency from the absorption edge (see figs. 4,5,6). Therefore in this chapter we calculate the polarization effect using the wave functions for arbitrary $\underline{k}$ given by Eqs. (3.15) and (3.16) with coefficients (3.20). We calculate first for the fundamental absorption and then for the inter-valence band absorption.

Summing Eq. (2.31) over the conduction band and valence bands, and using the matrix elements in Table I,we find

$$\alpha_{||}(k) = \frac{e^2}{\hbar c n} \sum_{i=1}^{3} \frac{p^2 k^2}{\hbar \omega_i \left| \frac{d(E_c - E_i)}{dk} \right|} \times \tag{5.1}$$

$$\int_0^\pi \{2(a_c c_i + c_c a_i)^2 \mathrm{Sin}\,\theta + [(a_c b_i - b_c a_i)^2 - 2(a_c c_i + c_c a_i)^2]\mathrm{Sin}^3\theta\} \times$$

$$\{f(E_i) - f(E_c)\} d\theta, \quad \text{and}$$

$$\alpha_{\perp} = \frac{e^2}{\hbar c n} \sum_{i=1}^{3} \frac{p^2 k^2}{\hbar \omega_i \left| \frac{d(E_c - E_i)}{dk} \right|} \times \tag{5.2}$$

$$\int_0^\pi \{[(a_c c_i + c_c a_i)^2 - \frac{(b_c a_i - a_c b_i)^2}{2}] \mathrm{Sin}^3\theta +$$

$$+ 2(b_c a_i - a_c b_i)^2 \mathrm{Sin}\,\theta\} \{f(E_i) - f(E_c)\} d\theta .$$

Fig. 3. Energy Bands

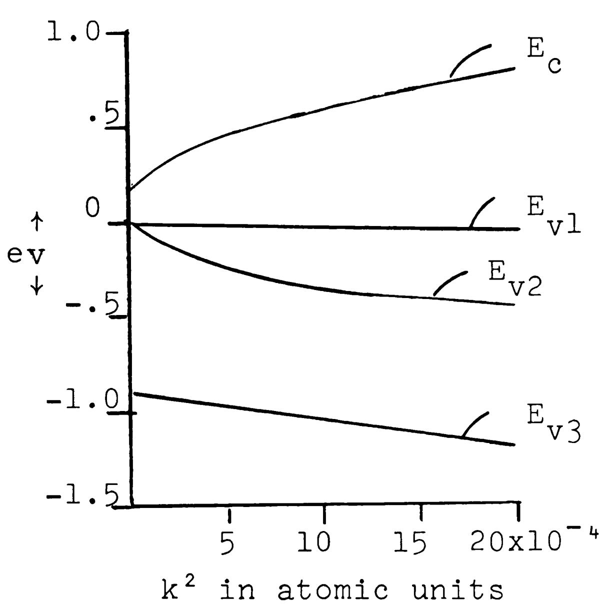
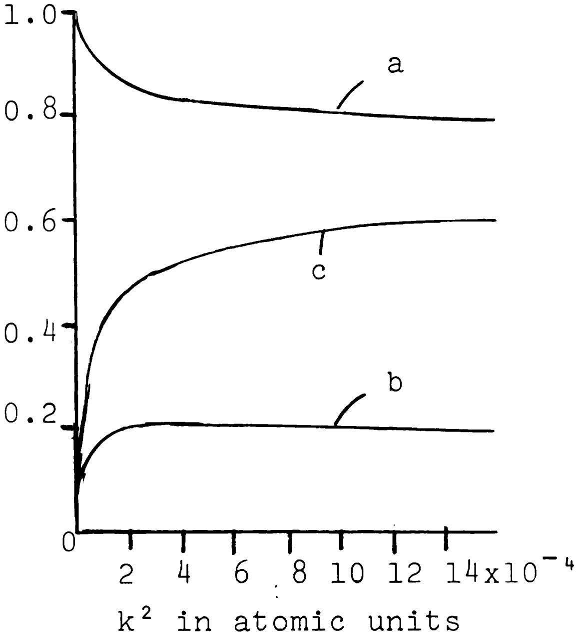


Fig. 4. Conduction Band



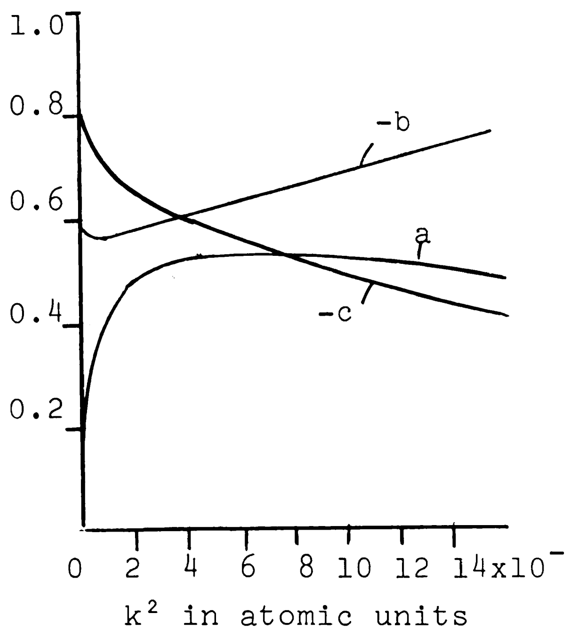


Fig. 5. Valence band two

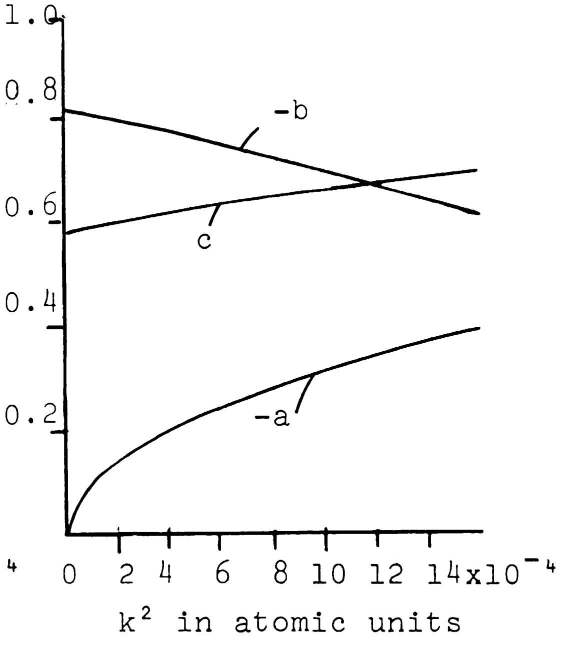


Fig. 6. Valence band three

Fig. 3. The energy bands for $m_1 = .54m$.

Figs. 4,5,6. Wave function coefficients for the energy bands of indium antimonide after Kane.[10]

where

$$\hbar\omega_i = E_c(k)-E_i(k), \tag{5.3}$$

and it is understood that

$$f(E_j) = f\,[E_j(k+d_j)]\;;\; j= c,i,2,3. \tag{5.4}$$

The energy bands are labeled just as in Chapter III and we have also used $a_1=0$ $b_1=0$, $c_1=0$.

We have written α as a function of k because it will be easier to calculate in this form. It is impractical to solve Eq. (3.4) analytically for arbitrary k, therefore we must solve it numerically. It is more efficient to find the three roots of Eq. (3.4) for several values of k, use the values to determine $\left|\frac{d(E_c - E_i)}{dk}\right|$ (approximately) for a certain k, then substitute this result and the proper $\hbar\omega_i$ for that k,found from Eq. (5.3), into the equation for α, than to choose a frequency ω and search for solutions of Eq. (3.4) that will satisfy Eq. (5.3). Having determined the coefficient multiplying the integral in the above manner, we than solve (3.4) again for $E_j(k+d_j)$, j=c,1,2,3,compute the distribution function and evaluate the integral numerically.

We should have used the term "corrected solutions to Eq. (3.4)" everywhere we mentioned the E_i"s above because the actual energies used are corrected for perturbations from higher bands as Kane showed[10]. These energies are shown in fig. 3 while the coefficients a_i,b_i,c_i as a function of k^2 are shown in figs. 4,5,6.

The computer program which performs all the operations described above is listed in the Appendix.

The polarization effect for the absorption due to the inter-valence band transitions is calculated in the same manner as that for the fundamental absorption. The matrix elements between the bands involved are calculated as they were for the fundamental absorption in Section 3.2. It may be noted that for this case the matrix elements, and thus the absorption and polarization effect, are all zero in the small k approximation, because according to Eqs. (3.21) and (3.16), none of the valence bands contain an S-like contribution in this limit, thus by selection rule (3.27) there can be no transitions. The solutions for $\alpha_{||}$ and $\alpha_{\perp}$ for arbitrary k can in this case be put in the same form as Eqs. (5.1) and (5.2) if we define

$$\hbar\omega_1 = E_1 - E_2; \ \hbar\omega_2 = E_1 - E_3; \ \hbar\omega_3 = E_2 - E_3, \qquad (5.6)$$

and for the first two terms of the sum change the subscripts according to the formula $c \rightarrow 1$, $1 \rightarrow 2$, $2 \rightarrow 3$ while for the third term we use the prescription, $c \rightarrow 2$. The resulting equations for $\alpha_{\perp}$ and $\alpha_{||}$ are solved numerically as before.

The parameters used in calculating the polarization effect for InSb are shown in Table II.

TABLE II

Parameters used in calculations for InSb.

$E_g = (.23-9.6 \times 10^{-5} \times T)$ ev $\quad m_c = .013 m E_g/.23$

$m_1 = .54m \quad m_2 = .015m \quad m_3 = .12m$

$\Delta = .9$ev $\quad P^2 = .44$ atomic units

$\mu_n = 7 \times 10^8 \times T^{-1.6}$ cm^2/v.sec $\quad \mu_p = 1.1 \times 10^8 \times T^{-2.1}$ cm^2/v.sec

The band parameters are as given by Kane [16] except E_g, m_c and m_1 which are as given by Ehrenreich [17]. The values of m_1 determined by various experiments are not consistent. We have chosen the value tabulated in preference to others because it is most defensible, and it also produces theoretical absorption versus photon energy curves closer to the experimental results. The mobilities vary with temperature and hole concentration and are as given in reference 18.

The results of the computations are given in terms of a dimensionless function we shall call the polarization effect coefficient, defined by

$$P_E = \frac{\alpha\| - \alpha\perp}{\alpha_{zero}}, \qquad (5.7)$$

where α_{zero} is the absorption at the temperature at which $\alpha\| - \alpha\perp$ is measured, for zero electric field.

Figure 7 shows the polarization effect coefficient for the fundamental absorption for intrinsic InSb, as a function of the photon energy, for $T = 300^{\circ}$K and $\underline{E}=100\mathrm{V}/_{\mathrm{cm}}$. The exact Fermi - Dirac distribution function was used in this case, not its Maxwellian limit as in Chapter III.

Fig. 8 shows the intra-valence band absorption at $T=300^{\circ}$K and $\underline{E}=100\ \mathrm{V}/_{\mathrm{cm}}$, which turns out to be much the same whether we use the intrinsic Fermi-Dirac distribution or go to the extrinsic case for a hole concentration of $4 \times 10^{15}/_{\mathrm{cm}^3}$ and a Maxwell Boltzmann distribution given by

$$\frac{4\pi^3 p\hbar^3 \exp(E/KT)}{(2\pi KT)^{3/2}(m_1{}^{3/2} + m_2{}^{3/2})} = f(E) \qquad (5.8)$$

where we have averaged over the highest valence band masses and p is the concentration of holes.

Fig. 9 shows P_E for inter-valence band absorption in extrinsic InSb at 77°K using the distribution Eq.(5.8), at various field strengths and hole concentrations. We note that the effect is much larger at the lower temperature. This is because the zero absorption does not change much over this temperature range because of the abundance of holes, but $\alpha_{||}-\alpha_{\perp}$ changes inversely with temperature.

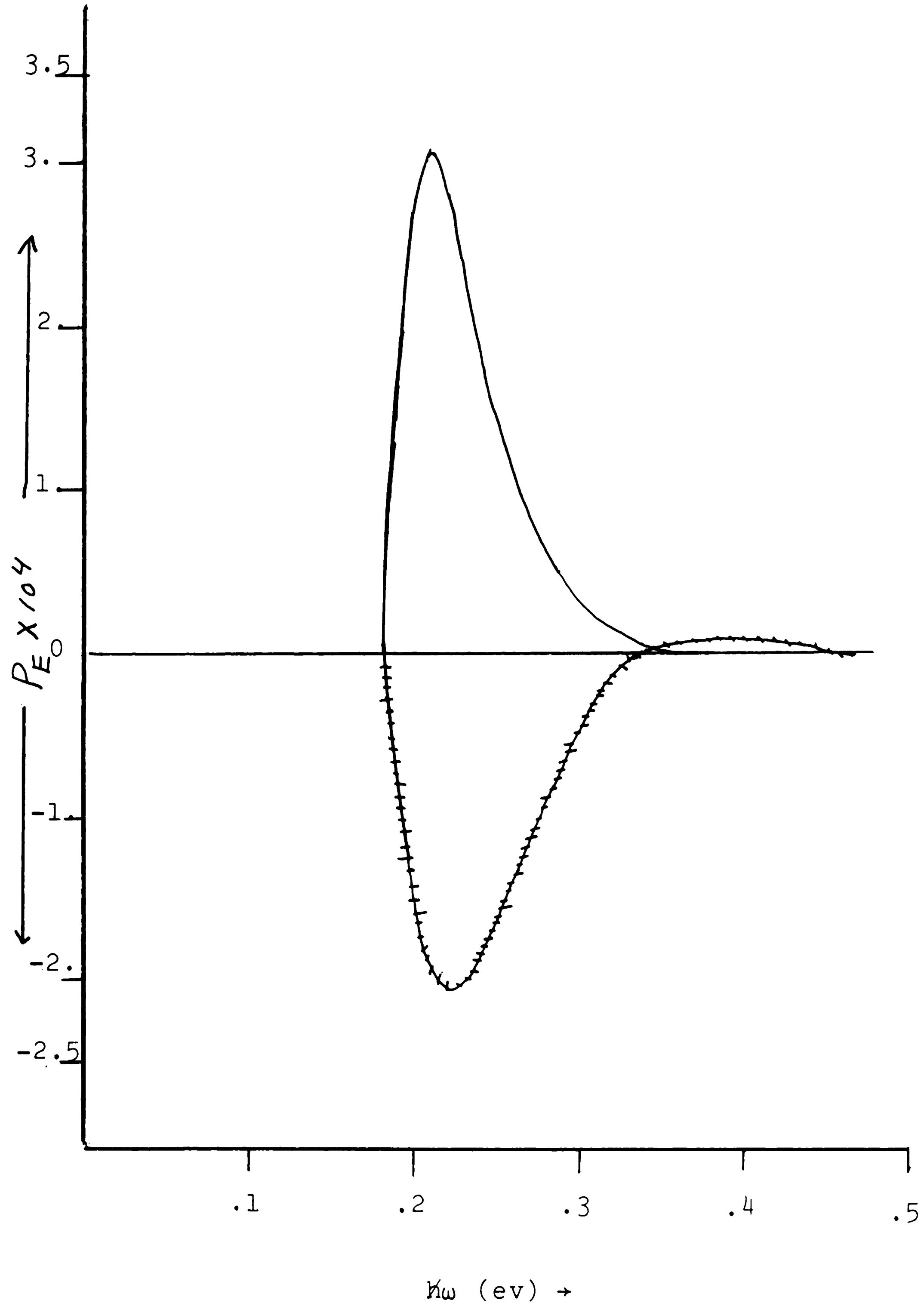


Fig. 7. Polarization coefficient versus energy for fundamental adsorption. $\underline{E}$=100V/cm T=300°K.

___ For first valence band to conduction band transitions.

+++ For second valence band to conduction band transitions.

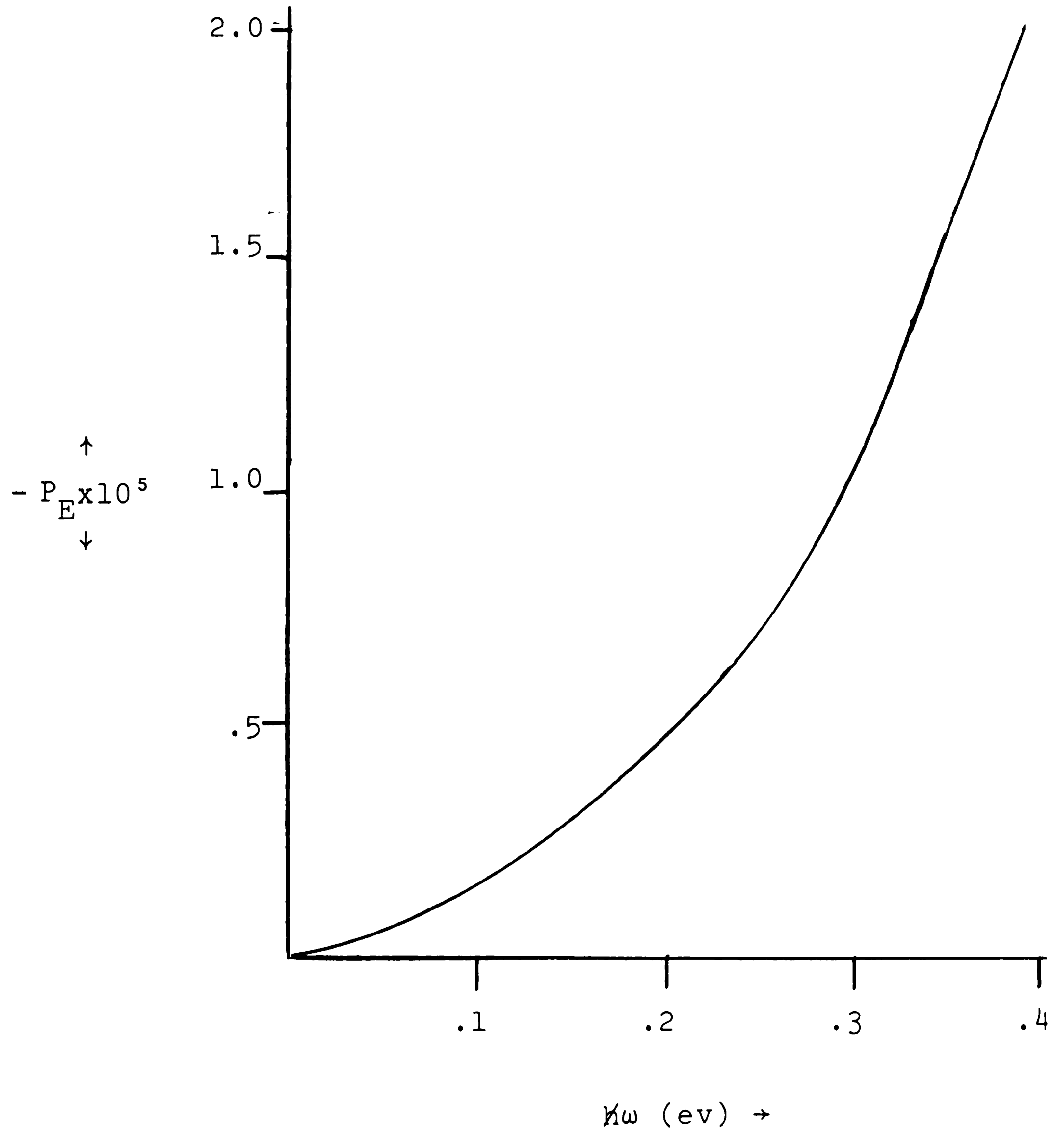


Fig. 8. The polarization effect for the intervalence band absorption (valence band two to valence band one transitions). T = 300°K, $\underline{E}$ = 100V/cm.

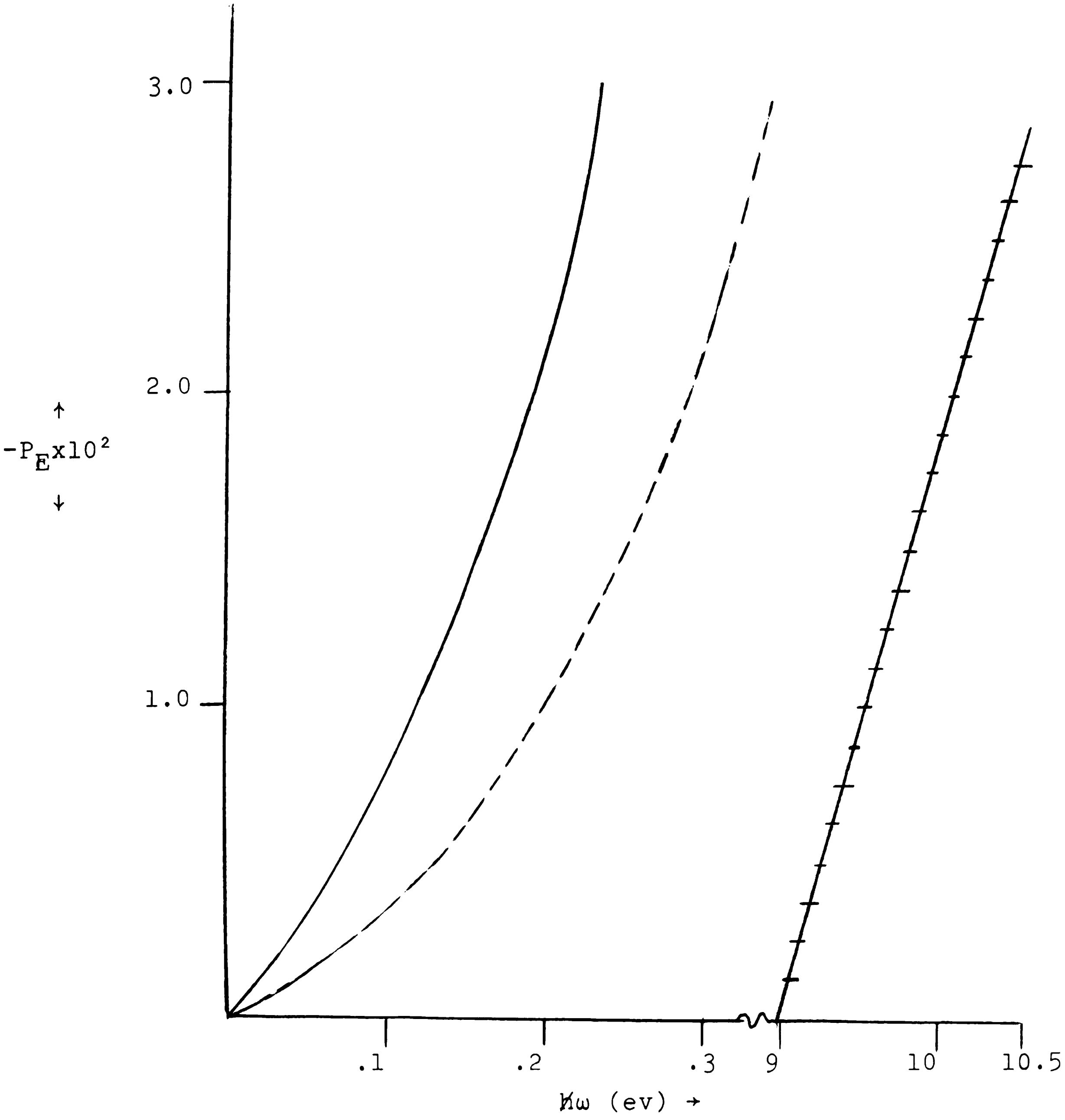


Fig. 9. The polarization effect for the inter-valence band absorption at 77°K; $\mu = 8x10^3$ cm²/V.sec, $p=4x10^{15}/cm^3$.

—— Valence band two to valence band one transitions, E=150V/cm.

--- Valence band two to valence band one transitions, E=100V/cm.

┼┼┼ Valence band three to valence band one transitions, E=100V/cm.

VI. DISCUSSION OF RESULTS

The behavior of the polarization effect coefficient curves we calculated in the last chapter, can be understood in detail using the principles discussed in Chapters III and IV. We next discuss each of the previously presented P_E-curves in turn, and point out how curves of this type can be used as experimental checks on the distribution function and wave functions involved.

1. Figure 7

The rapid rise and fall of the curve can be attributed to the fact that the Fermi function is changing rapidly in this region. The effect rises sharply near the absorption edge because the carriers are plentiful here. The fact that the effect rises from zero (and does not come down from infinity for example) is due to the fact that at slightly higher energies the Boltzmann like approximation is valid for the Fermi function and Eqs. (3.46) and (3.47) say the effect goes as k^2 in that region. The continuity of the equations results in the curve going to zero with k. However, before the true k^2 dependence sets in the number of carriers drops sharply and the effect (which is caused by the shift of these carriers with the electric field) drops with them.

The fact that the curve due to valence band one exhibits a simple positive peak while that due to valence band two goes negative, then positive, can be explained by the band structure. The first band has no Z or S component for any k. Thus the only transitions allowed are those between the X-like (or Y-like) functions in the valence band wave function and the S part of the conduction band function. As shown in Chapter IV, an X-like term produces a larger $\alpha_\perp$, and since the sign of the distribution factor is negative (see Chapter IV), we get a positive P_E.

Valence band two, however, has a dominant Z-like component near k=0 which together with the dominant S-like part of the conduction band leads to a negative polarization effect. Away from k=0,valence band two gains a rapidly increasing S-like part while its Z-like component decreases. In the conduction band almost the opposite happens. The S-like part decreases while the Z-like part increases rapidly. Thus the direction of the absorptions reverses with respect to the S and Z waves and therefore the sign of P_E must reverse.

Generally speaking this curve does not offer a good chance of checking the distribution functions and wave functions because the absorptions due to valence bands one and two overlap, therefore it would be hard to distinguish the effects of one from the other. However a slight amount of S-wave in the first valence band would bring the X-andZ-like parts of the conduction band into consideration which could significantly alter the total effect. Thus there are possibilites of using this kind of curve as a check on the S-content of the first valence band. The effect is small for this intrinsic case, but since the total absorption is large the absolute magnitude of $\alpha_{||} - \alpha_{\perp}$ is about .06/cm. We shall discuss this magnitude later with reference to other experiments. We have not discussed the third valence band transitions because the effect is insignificant in this case.

2. Figures 8 and 9 .

These figures involve transitions between the second and third valence bands and the first valence band. Because the first valence band contains no S-like part we can disregard the X-andZ-like parts of valence bands two and three. The absorption should therefore be characteristic of transitions between a higher X-band and a lower S-band except that the size of the latter increases with k (see figures 5 and 6). Approximation (3.31) is always good in the valence bands for intrinsic semiconductors, and for the extrinsic case we are using Eq. (5.8), therefore the Boltzmann form of the distribution function is valid for both cases. Also, the mobility in the valence bands is much smaller than that of the conduction band, therefore d is much smaller and approximation (3.43) is valid for much larger values of k. This is the same situation we discussed in Chapter III, therefore the results should be the same as for Eq. (3.46) except that since we are now considering transitions from a *higher* X-like band to a *lower* S-like band, the sign of the effect should be reversed. The figures show the required k^2 dependence. The curvature in the effect for valence band two is due to the curvature in this band as a function of k^2 . The masses of valence bands one and three are constant therefore $\hbar\omega \sim k^2$ and the curve is a straight line. Eventually, as k gets bigger, approximation (3.43) should become invalid, the number of holes should diminish and the effect should decrease. However at the higher values of k in these figures, the absorption has become so small that the effect would not be measurable.

Because the absorption spectra for the two transitions considered in figures 8 and 9 are widely separated, curves of this type should be a good test of the theory. Again a slight addition of some S-like part to valence band one would bring the X-like and Z-like parts of bands two and three into consideration and could change the effect considerably. Note the large change in P_E with $\underline{E}$. Changing $\underline{E}$ is equivalent to increasing the displacement of the distribution function. Thus this experiment should be a sensitive test of this displacement.

Earlier in the discussion we mentioned the absolute size of the polarization effect, $\alpha_{||}-\alpha_{\perp}$, for the fundamental absorption of the intrinsic semiconductor at 100V/cm was about .06/cm. The effect is also of a comparable magnitude for the extrinsic inter-valence band absorption at fields of 150V/cm (or larger), but elsewhere it is much smaller. The smallness of the absorption change suggests an experiment using the differential measurement technique.[19] Using this technique experimenters have measured modulations of the absorption due to a d.c. electric field to about .01/cm[20]. This measurement was for the fundamental absorption in silicon which is of the same order of magnitude as that in InSb, so if a like experiment could be arranged to measure P_E, in the above two situations it would involve a measurable effect. Instead of measuring the difference in the absorption between the field on and off situations, as was the case for the experiments referred to, one might measure the difference between the field parallel and the field perpendicular situations.

One could also hope to increase the absolute magnitude of the effect by doping,or the absolute and percentage-wise size by increasing the electric field. 150V/cm is near the limit where funny thingsstart happening to the mobility of InSb under normal circumstances, but a magnetic field greatly increases the size of the electric field one can apply before breakdown occurs. The effect of a magnetic field on the polarization effect considered here is not known.

It should be noted that the size of the effect measured in germanium by Pinson and Bray[8] and others[9] is considerably larger than in any of our theoretical curves (compare figures 10 and 11). Their effect was large enough to be measured without the sophistication of the differential technique.[21] Besides the facts that their measurements were made on a different material and at higher voltages than those for which our curves were drawn, there are several other possible reasons for this difference in magnitude.

We have not considered in our theory the heating of the electron population by the field. Since the absorption shifts toward higher energy and becomes broader with increasing temperature, heating could account for the shift and broadening of the experimental $\alpha\perp$ and $\alpha||$ curves. The heating would not change our analysis since we could account for it by simply changing the temperature in our calculations to match the shift in the experimental curves.

The heating does not explain the large size of the difference between the absorption parallel and absorption perpendicular measurements of Pinson and Bray. However the ratio of drift to thermal velocity in their experiment was about .5 while the largest value we used in the inter-valence band curves which correspond best to their experiment, was about .1. This difference amounts to increasing our field to 750V/cm (which is impossible, of course, for InSb without a magnetic field). Since the effect goes about as $\underline{E}^2$ this could account for

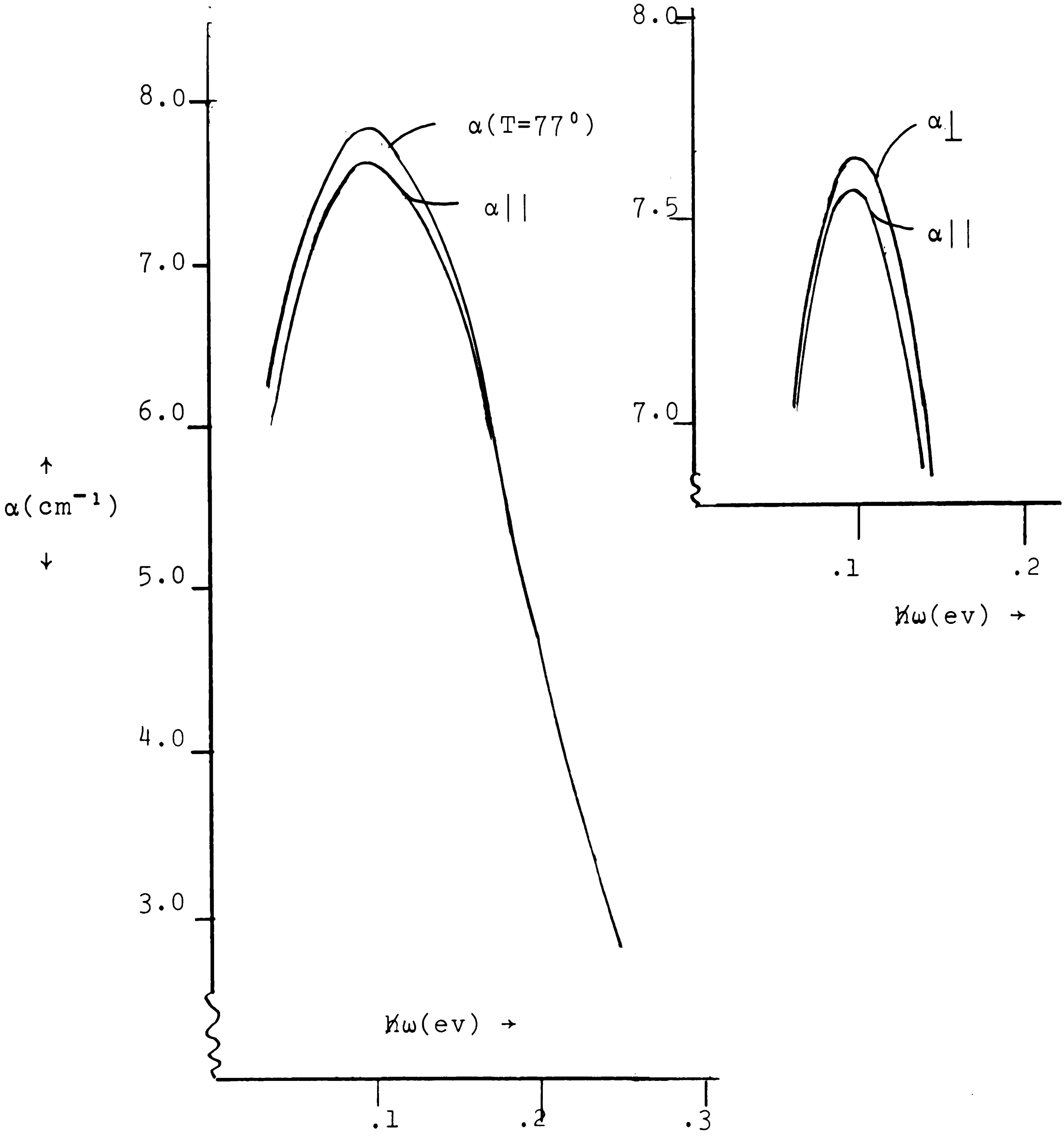


Fig. 10. The absorption for valence band two to valence band one transitions for indium antimonide; $T=77^{0}K$, $\mu=8x10^{3}cm^{2}/V.sec$, $p=4x10^{15}/cm^{3}$. Main figure shows absorption with zero field and $\alpha||$for $\underline{E}=150V/cm$. Inset shows $\alpha||$ and $\alpha\perp$ on expanded scale for $\underline{E}=150V/cm$.

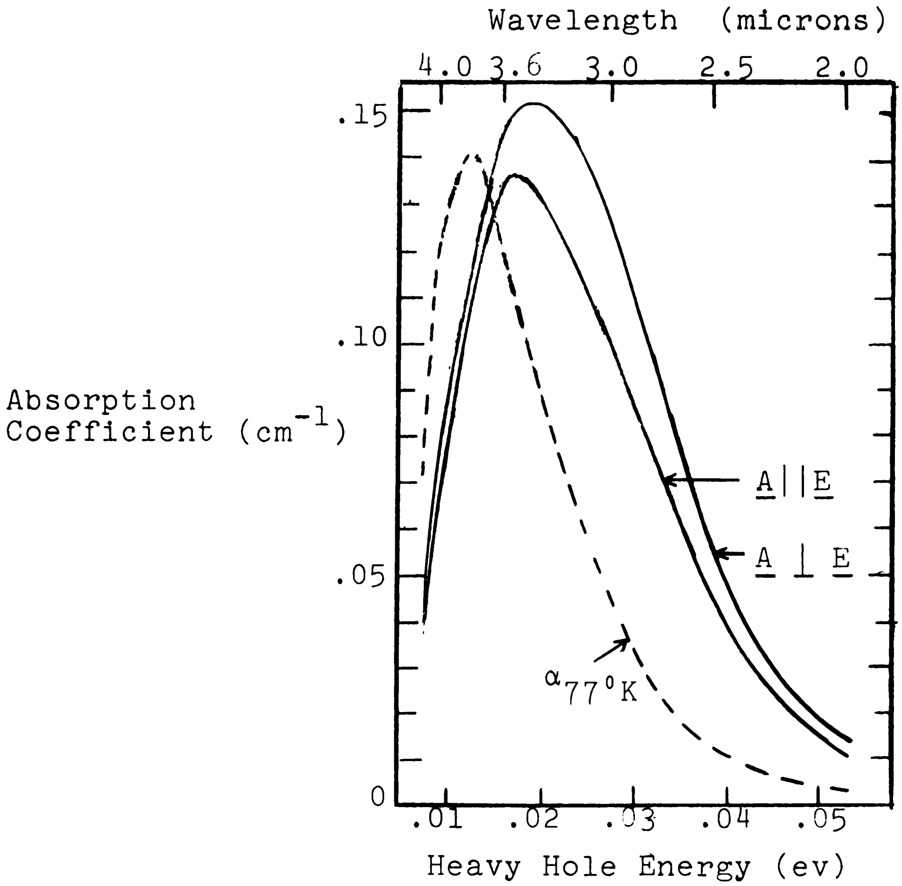


Fig. 11. Anisotropic absorption of polarized light by hot carriers in p-type germanium, for $\underline{E}$ = 760V/cm, T = 77°K, as measured by Pinson and Bray.[8]

the large size of the measured result.

Finally we mention what might possibly be the best use of this experiment. The method of numerical solution and programing for the theoretical calculation of this effect makes it quite easy to change distribution functions in the problem. One merely changes a few cards in the computer program. Thus one could, if he had some experimental data and had a fair idea of the wave function, substitute any distribution function he desired in the program - perphaps even insert an expansion of some kind and vary the parameters to fit the experimental curves. On the other hand if the wave functions of the material were not well understood, one could insert a rough distribution function and vary the coefficients of the wave function to try to match the general shape of the curve.

In general, given a distribution function, if the experimental results show a larger than predicted polarization effect, this indicates a greater disparity between the relative amounts of X and Z (or Y and Z) in the wave function for the band. A smaller than predicted effect indicates a more symmetrical arrangement of the distribution function, with the relative amounts of X,Y,Z more equal. The sign of the effect tells which is the greater, the X part or the Z part. Given a wave function, a larger effect means a more violently displaced distribution function. If for certain values of _k_ there are peculiarities in the distribution function, for instance an abnormal asymmetry, this will be reflected in an increase in the effect at that _k_.

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12. H is usually found by constructing a Lagrangian which gives the correct equations of motion as determined by the Lorentz force equations, then deriving the Hamiltonian from the Lagrangian. See J.H. VanVleck, Theory of Electric and Magnetic Suceptibilities (Oxford, The Clarendon Press, 1932) pp.7,20.

13. See for example, reference 11, (Schiff) pp. 249-250.

14. *Ibid*., p. 252.

15. In insulators the band structure does change. For a list of references on this subject see K.S. Viswanathan and J. Callaway, Phys, Rev. **143**, 564 (1966).

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21. It might be of some interest that it was the existence of the possibility of measurement of the polarization effect using the differential technique which prompted us to present a paper on this effect with T.O. Woodruff at the 1967 Chicago Meeting of the American Physical Society [see Bull of the Amer. Phys. Soc. 12. 405 (1967).] where we learned of references 7,8, 9 and related work.

APPENDIX

```
      PROGRAM POLEFF
C      PROGRAM WHICH CALCULATES THE POLARIZATION EFFECT

C     TO CHANGE THE DISTRIBUTION FUNCTION CHANGE CARDS WITH D IN
C     COLUMN ONE.
C     (NOT ALL CARDS HAVE TO BE CHANGED WITH ALL DISTRIBUTION
C     FUNCTIONS).

      COMMON/BLOCK1/EGAP,VMASS(4),DELTA
      COMMON/MAINAPZ/REFIND
D     COMMON/MAINABS/T,TK,EFERMI
      COMMON/MAINABR/EFIELD,SOBIL(4),NSR
      COMMON/MAINENS/SQP,CKANE,EGAPAD(4)
      T=300.
      DELTA=.9
      SQP=.44
      EGAPZERO=.23
      EGAP=EGAPZERO-9.6E-5*T
      EGAPT=.18
      EGAPAD(1)=.18-EGAP
      SOBIL(1)=7.E+8/(T**(1.6))
      DO 5 J=2,4
      EGAPAD(J)=0.
    5 SOBIL(J)=-1.1E+8/(T**(2.1))
      VMASS(1)=.013*EGAP/EGAPZERO
      VMASS(2)=-.015
      VMASS(3)=-.12
      VMASS(4)=-.54
      CKANE=2.*(1./VMASS(4)-1.)
      BOLTZC=8.61E-5
      TK=T*BOLTZC
D     EFERMI= EGAPT/2.+ 3.*TK*LOGF(-VMASS(4)/VMASS(1))/4.
      REFIND=3.96
      CALL ENERGY
      CALL ABSORBZ
      EFIELD=100.
      NSR=80
    7 FORMAT (5X,4HNSR=,I5)
      PRINT 7,NSR
    8 CALL ABPARPER
      END
```

```
      SUBROUTINE ENERGY
C     THIS SUBROUTINE FINDS THE E SUB K OF EQUATION(3.5) BY SOLVING EQ.
C     (3,4), THEN ADDING THE FREE ELECTRON ENERGY (EFREELEC) AND
C     CORRECTIONS FOR HIGHER BANDS (HPERT),

      COMMON/BLOCK1/EGAP,VMASS(4),DELTA
      COMMON/ENABS/SWV(102),A(4,102),B(4,102),C(4,102),EKANE(4,102),S(10
     12)
      COMMON/MAINENS/SQP,CKANE,EGAPAD(4)
      COMMON/ENERGYS/HHO2M,EPS,DD,DP,DB
      DIMENSION E(3),MI(3)
      HHO2M=(1,0544*6,582/(2,*9,108*5.2917*5,2917))*1.0E+3
      EPS=1,0E-9
      DD=DELTA-EGAP
      DP=DELTA*EGAP
      DB=DELTA*2,/3.
      E(1)=EGAP
      E(2)=0.
      E(3)=-DELTA
      SWV(1)=-1.0E-6
      PRINT 11,EGAP,DELTA,SQP,EPS,CKANE,EGAPAD(1)
   11 FORMAT (5X,5HEGAP=,F7,3,5X,6HDELTA=,F7.3,5X,4HSQP=,F7.3,5X,4HEPS=,
     1E10.2,5X,6HCKANE=,F8.2,5X,10HEGAPAD(C)=,F9,5)
      PRINT 12
   12 FORMAT (*0 K SQUARED IN ATOMIC UNITS.    ENERGY IN ELECTRON VOLTS.
     1    NI=NUMBER OF ITERATIONS FOR ENERGY I*)
      PRINT 13
   13 FORMAT(*0 K SQUARED        ENERGY(C)     ENERGY(V1)     ENERGY(V2)
     1 ENERGY(V3)       NC      NV2     NV3*)
      DO 75 K=2,102
      IF (K-22)18,18,20
   18 SWV(K)=SWV(K-1)+1.0E-6
      GO TO 22
   20 SWV(K)=SWV(K-1)+2.0E-5
   22 S(K)=SQP*SWV(K)*27,21*27.21
      EFREELEC=HHO2M*SWV(K)
      TA=DP*S(K)
      TB=DB*S(K)
      DO 65 J=1,3
      DO 45 L=1,10
      MI(J)=L
      FE=E(J)**3+DD*E(J)*E(J)-TA*E(J)-TB
      DFE=3,*E(J)*E(J)+2,*DD*E(J)-TA
      DELTAE=FE/DFE
      E(J)=E(J)-DELTAE
      IF (EPS-ABSF(DELTAE))45,55,55
   45 CONTINUE
   55 TF=E(J)+DB
      TG=E(J)-EGAP
      AN=(S(K)**,5)*TF
      BN=DB*TG/1,414214
      CN=TG*TF
      FNORM=(AN*AN+BN*BN+CN*CN)**,5
      A(J,K)=AN/FNORM
```

```
      B(J,K)=BN/FNORM
      C(J,K)=CN/FNORM
      HPERT=(B(J,K)*B(J,K)/2.+C(J,K)*C(J,K))*CKANE*EFREELEC
   65 EKANE(J,K)=E(J)+EFREELEC+HPERT+EGAPAD(J)
      EKANE(4,K)=EFREELEC/VMASS(4)+EGAPAD(4)
      A(4,K)=0.
      B(4,K)=1.
      C(4,K)=0.
  69  FORMAT (E13.3,4F14.9,3I7)
  75  PRINT 69,SWV(K),EKANE(1,K),EKANE(4,K),EKANE(2,K),EKANE(3,K),
     1MI(1),MI(2),MI(3)
      PRINT 81
  81  FORMAT (*0 K SQUARED        AC      BC        CC       AV2       BV2
     1     CV2       AV3      BV3      CV3*)
      DO 85 I=2,102
  83  FORMAT (E13.3,9F9.3)
  85  PRINT 83,SWV(I),A(1,I),B(1,I),C(1,I),A(2,I),B(2,I),C(2,I),A(3,I),B
     1(3,I),C(3,I)
      RETURN
      END
```

```
      SUBROUTINE ABPARPER
C     THIS SUBROUTINE CALCULATES THE ABSORPTION FOR A PARALLEL TO
C     E (ABSPAR) AND FOR A PERPENDICULAR TO E (ABSPER).  USING
C     THESE AND THE RESULTS OF SUBROUTINE ABSORBZ IT THEN
C     CALCULATES VARIOUS CURVES OF INTEREST.

      COMMON/BLOCK1/EGAP,VMASS(4),DELTA
D     COMMON/MAINABS/T,TK,EFERMI
      COMMON/MAINABR/EFIELD,SOBIL(4),NSR
      COMMON/ENABS/SWV(102),A(4,102),B(4,102),C(4,102),EKANE(4,102),S(10
     12)
      COMMON/ABSORPS/CNS,WV(102),DENOM(4,102),GA(4,102),GB(4,102),EPHOTO
     1N(4,102),ALPHA0(4,102),ABZERO(4,102)
      COMMON/ABRENGY/EZERO(3),ENTHETA(4)
      DIMENSION DRIFT(4),DRPLUSK(4),DISFUN(2,4),SUMS3(2,4),SUMS1(2,4),AR
     1EAS3(4),AREAS1(4),POLFEC(4,102),CHGPAR(4),CHGPER(4),X(2),CO(2),SI(
     22),FK(2,4),ABSPAR(4,102),ABSPER(4,102),POLFOA(4,102)
      RMASSE=9.108E-28
      HBAR=(1.0544/5.2917)*1.E-18
      DO 199 I=1,4
  199 DRIFT(I)=VMASS(I)*RMASSE*SOBIL(I)*EFIELD/HBAR
D 200 FORMAT (07H  TEMP=,F6.0,9H  EFERMI=,F8.5,9H  EFIELD=,F6.0,9H  EMOB
     1IL=,E12.4,9H  HMOBIL=,E12,4)
D     PRINT 200,T,EFERMI,EFIELD,SOBIL(1),SOBIL(2)
  201 FORMAT (07H CMASS=,F9.5,3X,7HV1MASS=,F9,5,3X,7HV2MASS=,F9.5,3X,7HV
     13MASS=F9.5,3X,9HDRIFT(C)=,E12.5,3X,10HDRIFT(V1)=,E12.5)
      PRINT 201,VMASS(1),VMASS(4),VMASS(2),VMASS(3),DRIFT(1),DRIFT(4)
  204 FORMAT (*0 KSQUARED      FK(ODD,C)   FK(EVEN,C)   FK(ODD,V1)   FK(O
     1DD,V2)  DISFUN(E,C)  DISFU(E,V1)  DISFU(E,V2)  ENTHETA(C)   ENTHET
     2A(V2)*)
      PRINT 204
      EZERO(1)=EGAP
      EZERO(2)=0.
      EZERO(3)=-DELTA
      DO 280 K=3,102
      DO 210 I=1,4
  210 DRPLUSK(I)=SWV(K)+DRIFT(I)*DRIFT(I)
      H=3.1415927/(2.*NSR)
      DO 215 N=1,2
      DO 214 J=2,4
      SUMS3(N,J)=0.
  214 SUMS1(N,J)=0.
  215 CONTINUE
      DO 260 IA=1,NSR
      X(1)=(2.*NSR+1.-2.*IA)*H
      X(2)=(2.*NSR-2.*IA)*H
      CO(1)=COSF(X(1))
      CO(2)=COSF(X(2))
      SI(1)=SINF(X(1))
      SI(2)=SINF(X(2))
      DO 250 J=1,4
      DO 240 N=1,2
      FK(N,J)=DRPLUSK(J)+2.*WV(K)*DRIFT(J)*CO(N)
      CALL ENGY(J,FK(N,J))
```

```
D 221 DISFUN(N,J)= 1./ (1. + EXPF((ENTHETA(J) - EFERMI)/TK))
      IF (J-1)240,240,224
  224 SUMS3(N,J)=SUMS3(N,J)+(SI(N)**3)*(DISFUN(N,J)-DISFUN(N,1))
      SUMS1(N,J)=SUMS1(N,J)+SI(N)*(DISFUN(N,J)-DISFUN(N,1))
  240 CONTINUE
  250 CONTINUE
  260 CONTINUE
      PROD=CNS*S(K)
      DO 270 J=2,4
      AREAS3(J)=H*(4.*SUMS3(1,J)+2.*SUMS3(2,J))/3.
      AREAS1(J)=H*(4.*SUMS1(1,J)+2.*SUMS1(2,J))/3.
      ABSPAR(J,K)=PROD*((GB(J,K)-2.*GA(J,K))*AREAS3(J)+2.*GA(J,K)*AREAS1
     1(J))/(EPHOTON(J,K)*DENOM(J,K))
      ABSPER(J,K)=PROD*((GA(J,K)-GB(J,K)/2.)*AREAS3(J)+GB(J,K)*AREAS1(J)
     1)/(EPHOTON(J,K)*DENOM(J,K))
  270 POLFEC(J,K)=ABSPAR(J,K)-ABSPER(J,K)
  279 FORMAT (E11.3,9E13.5)
  280 PRINT 279,SWV(K),FK(1,1),FK(2,1),FK(1,4),FK(1,2),DISFUN(2,1),DISFU
     1N(2,4),DISFUN(2,2),ENTHETA(1),ENTHETA(2)
  281 FORMAT (*0 KSQUARED IN ATOMIC UNITS,   EPHOTON IN EV,   ABSORPTION
     1S IN INVERSE CENTIMETERS*)
      PRINT 281
  282 FORMAT (*0 K SQUARED   EPHOTON(V1)  ABSPAR-ABSPER1   EPHOTON(V2)
     1ABSPAR-ABSRER2   EPHOTON(V3)  ABSPAR-ABSPER3*)
      PRINT 282
      DO 284 K=3,102
  283 FORMAT (E11.3,3(F14.7,E16.7))
  284 PRINT 283,SWV(K),EPHOTON(4,K),POLFEC(4,K),EPHOTON(2,K),POLFEC(2,K)
     1,EPHOTON(3,K),POLFEC(3,K)
  285 FORMAT (*0 EPHOTON(V1)     ABSPAR(V1)        ABSPER(V1)   EPHOTON(V2)
     1     ABSPAR(V2)        ABSPER(V2)   EPHOTON(V3)     ABSPAR(V3)        AB
     2SPER(V3)*)
      PRINT 285
      DO 290 K=3,102
  289 FORMAT (3(F12.7,2E16.7))
  290 PRINT 289,EPHOTON(4,K),ABSPAR(4,K),ABSPER(4,K),EPHOTON(2,K),ABSPAR
     1(2,K),ABSPER(2,K),EPHOTON(3,K),ABSPAR(3,K),ABSPER(3,K)
  292 FORMAT (*0 EPHOTON(V1)  CHANGEPAR(V1)   CHANGEPER(V1)  EPHOTON(V2)
     1  CHANGEPAR(V2)   CHANGEPER(V2)  EPHOTON(V3)  CHANGEPAR(V3)   CHAN
     2GEPER(V3)*)
      PRINT 292
      DO 299 K=3,101
      DO 294 J=2,4
      POLFOA(J,K)=POLFEC(J,K)/ABZERO(J,K)
      CHGPAR(J)=ABSPAR(J,K)-ABZERO(J,K)
  294 CHGPER(J)=ABSPER(J,K)-ABZERO(J,K)
  295 FORMAT (3(F12.7,2E16.6))
  299 PRINT 295,EPHOTON(4,K),CHGPAR(4),CHGPER(4),EPHOTON(2.K),CHGPAR(2),
     1CHGPER(2),EPHOTON(3,K),CHGPAR(3),CHGPER(3)
  300 FORMAT (*0 K SQUARED   EPHOTON(V1)  PAR-PEROABZERO1  EPHOTON(V2)
     1PAR-PEROABZERO2  EPHOTON(V3)  PAR-PEROABZERO3*)
      PRINT 300
      DO 304 K=3,101
  303 FORMAT (E11.3,3(F14.7,E16.7))
```

```
304 PRINT 303,SWV(K),EPHOTON(4,K),POLFOA(4,K),EPHOTON(2,K),POLFOA(2,K)
   1,EPHOTON(3,K),POLFOA(3,K)
    RETURN
    END
```

```
      SUBROUTINE ENGY(I,FK)
C     THIS SUBROUTINE CALCULATES VALUES OF E(K+D),(ENTHETA),CALLED FOR
C     BY SUBROUTINE ABPARPER.

      COMMON/BLOCK1/EGAP,VMASS(4),DELTA
      COMMON/ENERGYS/HHO2M,EPS,DD,DP,DB
      COMMON/ABRENGY/EZERO(3),ENTHETA(4)
      COMMON/MAINENS/SQP,CKANE,EGAPAD(4)
      EFREELEC=HHO2M*FK
      IF(4-I)320,320,325
  320 ENTHETA(4)=EFREELEC/VMASS(4)+EGAPAD(4)
      GO TO 365
  325 S=SQP*FK*27.21*27.21
      TA=DP*S
      TB=DB*S
      DO 345 L=1,20
      FE=EZERO(I)**3+DD*EZERO(I)*EZERO(I)-TA*EZERO(I)-TB
      DFE=3.*EZERO(I)*EZERO(I)+2.*DD*EZERO(I)-TA
      DELTAE=FE/DFE
      EZERO(I)=EZERO(I)-DELTAE
      IF(EPS-ABSF(DELTAE))345,355,355
  345 CONTINUE
  355 TF=EZERO(I)+DB
      TG=EZERO(I)-EGAP
      AN=(S**.5)*TF
      BN=DB*TG/1.414214
      CN=TG*TF
      FNORM=(AN*AN+BN*BN+CN*CN)**.5
      B=BN/FNORM
      C=CN/FNORM
      HPERT=(B*B/2.+C*C)*CKANE*EFREELEC
      ENTHETA(I)=EZERO(I)+EFREELEC+HPERT+EGAPAD(I)
  365 RETURN
      END
```