

A MAGNETOREFLECTION STUDY OF ARSENIC AND BISMUTH

by

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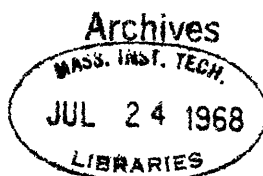
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ABSTRACT

We have studied the band structure of the semimetals, arsenic, and bismuth, using the magnetoreflexion technique. In arsenic, two new series of oscillations in the magnetoreflexivity have been found. One series of oscillations, observed when the magnetic field is perpendicular to the trigonal axis, seems to be associated with direct interband transitions between two bands with a critical point at T in the Brillouin zone. It was found that the band structure at T given by the pseudopotential calculation of Lin and Falicov is not consistent with these experimental results. We also found that there may be a very small pocket of carriers at T associated with the bands under discussion. No effects due to such a pocket have been previously observed, however; perhaps because of the very small number of carriers involved.

A second series of oscillations is observed when the magnetic field is parallel to the trigonal axis. We have associated these oscillations with direct interband transitions between two bands with a critical point along the Q axis in the Brillouin zone, where we are using the symmetry notation of Lin and Falicov. In this case, we concluded that our experimental results were consistent with the band structure at Q predicted by the Lin-Falicov calculation. The lineshape of the observed oscillations was found to be unusual, but by extending the calculations of Dresselhaus and Dresselhaus, and Roth, Lax and Zwerdling, we were also able to understand this peculiar lineshape in terms of the band model of Lin and Falicov.

Oscillations in the magnetoreflexivity were also observed for bismuth. These oscillations are associated with direct interband transitions between the valence and electronic conduction bands, which have a critical point at L in the Brillouin zone. When the magnetic field is along the binary or bisectrix axes, the oscillations we observe are in good agreement with the oscillations previously observed by Brown, Mavroides and Lax, and the relation between the resonance fields and photon energies is found to be accurately described by the two band

model of Lax. When the magnetic field is along the trigonal axis, however, small oscillations in the reflectivity can be seen which have not been previously reported. These oscillations also seem to be associated with transitions between the valence and conduction bands, and have resonance fields and photon energies which are also accurately described by the Lax model.

We also calculated the lineshape of the oscillations in the magnetorefectivity, using the Lax model. We used the one electron density matrix technique to calculate the conductivity, including all of the nonparabolic effects predicted by the Lax model, and then used conventional electromagnetic theory to find the reflectivity. We found that there was reasonably good agreement between theory and experiment for the oscillations associated with interband transitions, but that the agreement between theory and experiment was very poor for the cyclotron resonance lineshape. We were then able to explain most of these discrepancies by considering the departures from the Lax model due to the interaction of the valence and conduction bands with the other bands nearby (the Baraff interaction.) As a result of this work, we were able to develop a relatively simple band model for the valence and conduction bands in bismuth which includes the effects of the Baraff interaction to first order in perturbation theory, and is therefore considerably more accurate than the Lax model. Furthermore, this model also seems to explain most of the relevant magnetoreflexion, de Haas-van Alphen and cyclotron resonance data.

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Figure	$\hbar\omega$ (eV)	n_1	n_2	S_1	S_2	j_1	j_2	D_1	D_2
a.	.1534	1	2	1	1	1	2	-1	1
b.	.1534	1	1	1	-1	1	2	-1	1
c.	.06908	0	1	1	1	0	1	-1	1
d.	.06908	0	0	1	-1	0	1	-1	1
e.	.05816	0	1	1	1	0	1	1	1
f.	.05816	0	0	1	-1	0	1	1	1

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a. Velocity matrix elements involving the $j=0$ Landau level. The quantum numbers for each of the transitions displayed are:

Transition type	j_1	j_2	S_1	S_2	D_1	D_2
anomalous spin conserving	0	1	1	1	-1	1
anomalous spin flipping	0	1	1	-1	-1	1
intraband spin conserving	0	1	1	1	1	1
intraband spin flipping	0	1	1	-1	1	1

b. Velocity matrix elements not involving the $j=0$ Landau level. In this case, each graph is the sum of several interband transitions degenerate in the Baraff model. (See Text.) The quantum numbers of the transitions associated with each graph are:

Transition type	j_1	j_2	S_1	S_2	D_1	D_2
normal spin conserving	1	2	1	1	1	-1
	1	2	1	1	-1	1
	1	2	-1	-1	1	-1
	1	2	-1	-1	-1	1
spin flipping shifted up	1	2	1	-1	-1	1
	1	2	-1	1	1	-1
spin flipping shifted down	1	2	1	-1	1	-1
	1	2	-1	1	-1	1

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INTRODUCTION

The group V semimetals, bismuth, arsenic, and antimony, have long been of considerable interest to solid state physicists because of the striking diamagnetic and magneto-oscillatory phenomena which they display.⁽¹⁾ Bismuth, for example, for which the de Haas-van Alphen effect is quite large, was the first material to be studied by this technique.⁽²⁾ The reasons for these large diamagnetic and magneto-oscillatory effects are the small effective masses and Fermi energies of these materials.

Unfortunately, the DHVA and related effects only provide information about the energy bands at the Fermi surface, and for these materials the Fermi surface only involves a small region of the Brillouin zone.

On the other hand, interband magnetoreflexion experiments have been found to be very useful in studying the band structures of the semimetals at energies up to several tenths of an electron volt away from the Fermi level.⁽³⁻⁵⁾ In these experiments, we study those oscillations in the infra-red reflectivity at high magnetic fields which are associated with direct interband transitions from occupied Landau levels in one band to unoccupied Landau levels in another one. By studying these oscillations as a function of photon energy and polarization of the light, and magnetic field magnitude and orientation, one can get some very detailed information about the bands involved in the transition. An example of such a study was one carried out by Brown et al.⁽³⁾ on bismuth, which clearly established the non-parabolic nature of the strongly coupled conduction and valence bands.

In this thesis is described an interband magnetoreflexion study of the semimetals, bismuth and arsenic, using a somewhat improved version of the

equipment and techniques of Brown et al. Both materials were studied to demonstrate the two complementary aspects of an interband magnetoreflexion study. In arsenic, we have an example of a material which has never been studied before by the magnetoreflexion technique, and we will see how our experiments yield additional information not available from DHVA⁽⁶⁾ or CR⁽⁷⁻⁸⁾ measurements. Bismuth, on the other hand, is an example of a material that has been studied so extensively^(9,21) that we can attempt to calculate the reflectivity as a function of photon energy and magnetic field directly from the proposed band model.⁽¹⁰⁾ This allows us to both check the adequacy of the band model, and also extract more information out of our experimental results than we could have obtained using a less detailed theory.

In this thesis, we will first discuss bismuth because its properties are well enough understood so that we may profitably discuss our magnetoreflexion measurements in very great detail. In the first chapter, we will begin by presenting some of the pertinent experimental and theoretical studies of bismuth which have been reported in the literature. We will also describe the A_7 crystal structure which is characteristic of all the group V semimetals.⁽¹¹⁾ In the second chapter, we will present and discuss the results of our experiments on bismuth, which are essentially consistent with those of Brown et al.⁽³⁾ In the third chapter, we will calculate the optical reflectivity of bismuth in a magnetic field, taking into account the non-parabolic nature of the coupled conduction and valence bands associated with the electrons. This is the first time that the magnetoreflexion lineshape has been calculated in a consistent way for non-parabolic, strongly coupled bands, and qualitative agreement between theory and experiment has been obtained. Perhaps the most important result of

the lineshape calculation, however, was that it enabled us to obtain a greatly improved model for the structure of the strongly coupled electron and valence bands in bismuth.

In the final chapter, we will discuss the results of the very fruitful magnetoreflexion experiments on arsenic. In the light of these results, we will also consider the band model of Lin and Falicov,⁽¹²⁾ which was calculated by the pseudopotential technique, with the parameters in the pseudopotential chosen to give a fit to previous DHVA⁽⁶⁾ experiments. Some striking discrepancies have been found.

CHAPTER I

BISMUTH

Background Material

In this chapter we will discuss some experimental studies which have contributed to our understanding of the band structure of bismuth. We will also briefly treat those theoretical developments necessary to understand the experiments. We will begin by describing the crystal structure of bismuth in Section A. In Section B we will discuss some of the pertinent experimental and theoretical work which has been reported in the literature.

SECTION IA

Crystal Structure

Bismuth has the A_7 crystal structure, characteristic of all the group V semimetals.⁽¹¹⁾ This crystal structure can be thought of as a small distortion from the simple cubic (SC) lattice. To understand this distortion, we will look at the SC lattice as consisting of two interpenetrating fcc lattices. These two lattices would be arranged in the same way as the interpenetrating fcc sodium and chlorine lattices are arranged in the rock-salt structure.

The first distortion we must make is to translate one fcc lattice slightly with respect to the other along the body diagonal of the cube. We now have a fcc lattice with two atoms and 10 electrons per unit cell, which could be either a semiconductor or a semimetal.⁽¹³⁾ The second distortion is a rhombohedral shear, which is a stretching of the crystal structure along the same body diagonal as was involved in the displacement. This body diagonal now becomes the trigonal axis of the system. The resultant A_7 structure has the Brillouin zone shown in Figure 1, which has the shape of a squashed truncated

octahedron. In this figure, there are three binary axes parallel to the three TW axes in the Brillouin zone, and three bisectrix axes lying in the three mirror planes. The ones explicitly indicated in Figure 1 are the crystalline axes perpendicular to the sample faces. In the future, whenever we require a coordinate system (to display an effective mass tensor, for example), we will align it with respect to these crystalline axes, with the x, y and z coordinates parallel to the binary, bisectrix, and trigonal axes, respectively.

Due to the low symmetry of the A_7 structure, band calculations are very difficult for these materials. Bismuth, where the spin orbit splitting is too large to be considered as a small perturbation,⁽¹⁴⁾ is particularly hard to handle. Furthermore, as in all the group V semimetals, there are small band gaps and effective masses near the Fermi surface, and it would take an accuracy far greater than that claimed by present first-principal band calculations to predict them. All band calculations do show, however,^(11,14-16,83) that in general, the rhombohedral shear, which makes the L and T points non-equivalent, tends to raise the bands at T and lower the bands at L, so it is thought that there are electrons near L and holes near T for all of these materials. Because of our special interest in the L points, we will find it convenient to define the principal L point as the one lying in the mirror plane perpendicular to the binary axis of the sample (i.e. the axis perpendicular to the binary optical face.) The other two L points will be known as the nonprincipal ones.

SECTION IB

Results of Previous Work

Early work

The de Haas-van Alphen effect was first discovered in bismuth in 1930.⁽²⁾ Subsequent studies using both the DHVA⁽¹⁷⁻¹⁹⁾ and other related effects,⁽²⁰⁻²¹⁾ and cyclotron resonance experiments,⁽²²⁻²⁴⁾ have shown that these oscillations are due to roughly ellipsoidal* pockets of electrons in the Brillouin zone. These experiments, when coupled with the arguments of Section IA, were able to greatly restrict the number of possible arrangements of the electron pockets in the Brillouin zone, but could not completely determine the correct one.

In 1960, Cohen and Blount⁽²⁵⁾ noted that the peculiar phase⁽²⁶⁾ of the DHVA oscillations in bismuth implied that the Landau level separation was equal to the spin splitting. They were able to explain this peculiarity by assuming that the curvature of the conduction band was essentially determined by its strong interaction with a single valence band, separated from it by a small energy gap. At about the same time, magnetoreflexion oscillations associated with transitions across this small gap were experimentally observed.^(27,57)

THE DRESSELHAUS MAGNETOREFLECTIVITY CALCULATION

The results of the preliminary magnetoreflexion studies prompted Dresselhaus and Dresselhaus⁽²⁸⁾ to calculate the lineshape of the oscillations in the magnetoreflexivity which would be expected for a simple band model in the presence of free carriers.⁽²⁹⁾ The effects they considered

* The ellipsoidal nature of the Fermi surface has been definitely established only recently. For further discussion of this point, see Section IIIE,

were due to direct interband transitions between Landau levels in two spherically symmetric bands with quadratic energy dependence and extrema at the same point in the Brillouin zone. The effects of spin were ignored. We will present some of their results in some detail to explain how one can obtain information about the band structure from a magnetoreflexion experiment. Three of their conclusions are especially pertinent.

First, it was found that for their model, interband transitions are allowed only between states with the same Landau level index. The simplicity of this selection rule is a consequence of both the coincidence of the two band extrema in the Brillouin zone and the simple nature of the effective mass tensors. In particular, if the two bands were not coincident, the selection rules would not only be much more complicated, but they would also be functions of the magnetic field.* No such complications were observed in the magnetoreflexion data, which strongly supports the idea that the electron ellipsoids are three in number, and centered right at the L points in the Brillouin zone, where the coincidence of the band extrema is required by symmetry,⁽³¹⁾ rather than 6 in number, and located in the vicinity of the L points as had been previously assumed.⁽³²⁾ The three ellipsoid model has subsequently been supported by a number of other experiments.⁽³³⁻³⁴⁾

Secondly, the Dresselhaus calculation shows that there are oscillations in both the real and imaginary parts of the conductivity. If the relaxation time is relatively long, the sharp peaks of these oscillations occur at fields very close to what we will call the critical fields. A critical field is one at which there is a peak in the joint density of states for allowed transitions

* See Reference 30 and Appendix A for further details.

between Landau levels at an energy equal to that of the incident photons. If we use the parabolic band model under discussion to treat interband transitions, this critical condition becomes

$$\hbar\omega_{\text{res}} = |E_a(n,0) - E_b(n,0)| \quad (IB1)$$

where $E_j(n, k_H)$ is the energy of Landau level n in band j ; and $\hbar k_H$ is the component of the crystal momentum parallel to the magnetic field. The Landau level energy is

$$E_j(n, k_H) = E_j^0 + \frac{\hbar e H}{m_o m_j^* c} \left(n + \frac{1}{2}\right) + \frac{\hbar^2 k_H^2}{2m_{Hj}^* m_o} \quad (IB2)$$

where E_j^0 , m_j^* , m_{Hj}^* and m_o are respectively: the energy at the band extremum, the cyclotron effective mass, the effective mass parallel to the magnetic field for band j , and the free electron mass. The reflectivity itself is a complicated function of the total conductivity, including the free carrier terms, but well above the plasma frequency it was found that the peak in the conductivity corresponds to a peak in the reflectivity. The lineshape is asymmetric due to asymmetries in the real and imaginary parts of the conductivity. If we plot the magnetic fields at the reflectivity peaks as a function of photon energy, E_{ph} , (a "fan chart") the points will therefore be arranged in a series of straight lines described by the equation

$$E_{ph} = E_g + \frac{\hbar e H}{m_o c m_r^*} \left(n + \frac{1}{2}\right) \quad (IB3)$$

where
$$\frac{1}{m_r^*} = \frac{1}{m_a^*} + \frac{1}{m_b^*} \quad (IB4)$$

and m_a^* and m_b^* are the cyclotron effective masses for bands a and b. In an experiment the quantities which could be determined from the fan chart are E_g , the energy gap, and m_r^* , the reduced cyclotron effective mass.

Finally, it was found that the entire interband contribution to the conductivity is proportional to the quantity $|\langle U_a | v_i | U_b \rangle|^2$ where U_a and U_b are the band edge wave functions for the two bands (the wave functions at the extrema) and v_i is the component of the velocity operator parallel to the electric field. By using polarized light, we can find the relative magnitudes of the different vector components of the velocity matrix element coupling the bands, and thus get information about the symmetry types of the bands involved in the transition.

Thus we see that the magnetoreflexion experiments give us a considerable amount of very detailed information about the bands involved in the interband transition.

The lineshapes calculated by Dresselhaus and Dresselhaus were found to be in satisfactory agreement with those obtained in the preliminary magnetoreflexion experiments.⁽²⁷⁾

EXPERIMENTS OF BROWN, MAVROIDES AND LAX

These preliminary experiments were followed by a more complete study covering a greater range of magnetic fields and photon energies.⁽³⁾ For the first time the oscillation of lowest quantum number ($n=0$) was observed.

When the magnetic fields at the reflectivity peaks were plotted against the photon energy for these more extensive experiments, the lines of the fan chart were seen to be decidedly curved, indicating that the bands were not parabolic at all. Furthermore, the lineshape of the $n=0$ resonance was seen

to be quite different from that of the other oscillations, which had the shape predicted by the Dresselhaus calculation.

Though the situation in bismuth was clearly more complicated than the situation considered in the Dresselhaus calculation, Brown, Mavroides and Lax⁽³⁾ made the reasonable assumption that the resonance field, experimentally defined as that field at which there was a peak in the reflectivity, would still correspond closely to a critical field. The lineshape calculation of Chapter III shows that this is, in fact, correct for all the interband oscillations, including the strangely shaped one with $n=0$.

It was found that an excellent fit to the data could be obtained by calculating the critical fields using the selection rules and Landau level energies appropriate to the two band model of Lax.^(25,35) In this model, one assumes that the properties of the valence and conduction bands are completely determined by the strong interaction between them, and finds for the zero field dispersion relation

$$E_c(\vec{k}) = -E_v(\vec{k}) = \sqrt{\frac{E_g^2}{4} + E_g \vec{k} \cdot \frac{\vec{\alpha}}{2m_0} \cdot \vec{k}} \quad (\text{IB5})$$

where c and v label conduction and valence bands, respectively. The tensor $\vec{\alpha} = (\vec{m}^*)^{-1}$ describes the curvature at the bottom of the band, as is seen by expanding the square root to find

$$E_c(\vec{k}) = -E_v(\vec{k}) \sim \frac{E_g}{2} + \vec{k} \cdot \frac{\vec{\alpha}}{2m_0} \cdot \vec{k} \quad (\text{IB6})$$

if

$$\frac{\vec{k} \cdot \vec{\alpha} \cdot \vec{k}}{2m_0} \ll \frac{E_g}{2} \quad (\text{IB7})$$

In the Lax model the constant energy surfaces are ellipsoidal, though non-parabolic. (See Equation IB5)

The corresponding Landau level energies are

$$E_c(n, s, k_H) = \sqrt{\frac{E_g^2}{4} + \frac{E_g}{2} (\beta^* H [2n+1-s] + \frac{\hbar^2 k_H^2}{m_o m_H})} \quad (1B8a)$$

and

$$E_c(n, s, k_H) = -E_v(n, s, k_H) \quad , \quad (1B8b)$$

where

$$m_H = \frac{\vec{H} \cdot \vec{m}^* \cdot \vec{H}}{H^2} \quad , \quad (1B9a)$$

$$\beta^* H = \frac{\hbar e}{m_o c} \frac{(\vec{H} \cdot \vec{m}^* \cdot \vec{H})^{1/2}}{|\vec{m}^*|^{1/2}} \quad (1B9b)$$

the symbol $|\vec{m}^*|$ means the determinant of the matrix $\vec{m}^*$, and $s = \pm 1$ is the spin quantum number.* Note that, according to this model, the Landau level of energy $E(n, s=-1, k_H)$ is degenerate with the Landau level of energy $E(n+1, s=1, k_H)$. Once again $\vec{m}^*$ is defined by the curvature of the bands at the energy extremum, and not at the Fermi level.

The selection rules used by Brown et. al.⁽³⁾ were $\Delta n = 0$, and $\Delta S = 2$, so that the critical condition was

$$\hbar\omega_{res.} = E_c(n, 1, 0) - E_v(n, -1, 0) \quad (1B10)$$

though there are many other transitions which are also allowed,⁽¹⁰⁾ which are degenerate with this one. In Table 1, we give the values of E_g , β^* and $E_g \beta^*$, which were used by Brown et. al. to fit their data. In this table, we also give the results of several other recent determinations of the band parameters of bismuth.

*Note that the zero of energy and the sign of the spin term are consistent with the definitions of Chapter III, and are not the same as those used by Brown et. al.

SPLITTING OF LANDAU LEVELS

Although this model does give an excellent fit to the magnetoreflexion data, it had been known for some time that the Landau levels were really not degenerate.^(36,98,99) Extensive measurements of this splitting were made by Smith, Baraff, and Rowell⁽³⁷⁾ using DHS techniques; and by Mase,⁽³⁸⁾ who observed the giant quantum oscillations in the magnetoacoustical attenuation. These experiments give essentially the same data as a DHVA experiment, but with much higher resolution. The values measured for the splitting were on the order of 5 or 10% of the total Landau level spacing.

This small but significant departure from the Lax model occurs because the tightly coupled conduction and valence bands do interact with other energy bands nearby. Various experimentalists⁽³⁷⁻³⁸⁾ have taken this into account by replacing the expression $2n+1 - s$, which occurs in the Lax formula with the expression $2n+1 - \gamma s$ where γ is a constant of order unity. There is no theoretical justification for this procedure.⁽³⁹⁾

Baraff, on the other hand, has considered the effects of the rest of the band structure on the two bands of the Lax model in the lowest order of perturbation theory.⁽³⁹⁾ His final expressions are a bit unwieldy, but we have found that the results of the magnetoreflexion experiments indicate that his expressions may be greatly simplified.

From his results, it appears that: a) the energies of the Landau levels can be significantly shifted from the values predicted by the Lax model; and b) the degeneracy predicted by the Lax model may be lifted; but c) the energy shifts are such that the cyclotron resonance frequency and the resonant fields and photon energies for interband transitions will still be accurately given by the Lax formulas; though d) the lineshape of the oscillations may differ

somewhat from those predicted by the Lax model. We will discuss these points in more detail in Chapters II and III.

To summarize the experimental situation with respect to the electrons, it may be said that the band structure for the electrons is well understood to zeroth order, and that recent studies are starting to give information about the first order corrections to the energy. The Fermi surface for the electrons consists of three pieces, which are approximately elongated prolate ellipsoids,^(40,64) each one centered about one of the L points in the Brillouin zone, with its long axis tilted about 6° away from the bisectrix axis in the bisectrix-trigonal plane.

THE HOLE BAND

The story of the hole band in bismuth is considerably shorter. The first detailed information about the hole Fermi surface came from a series of cyclotron resonance measurements,^(22,24,41) the first of which was performed in 1955.⁽⁴¹⁾ These experiments showed that the hole Fermi surface was an ellipsoid of revolution, which implied that the band extremum was along the trigonal axis of the Brillouin zone.

DHVA oscillations due to the holes were not observed until 1960.⁽⁴²⁾ These carriers have much larger effective masses than the electrons, so that the experiment has to be performed at very low temperatures, between $.06^\circ$ and $.1^\circ\text{K}$, for the DHVA oscillations to be observable by the conventional torque balance technique. Subsequent experiments⁽⁴⁰⁾ have shown that the volume of the hole ellipsoid agrees very well with the total volume of the three electron ellipsoids, indicating that there is one hole ellipsoid at T, and that there are no other pieces of Fermi surface to be accounted for.⁽³⁴⁾ No indications of a nonparabolic dispersion relation have ever been found for the holes.

The g factor of the holes in bismuth was first measured by Smith, Baraff, and Rowell⁽³⁷⁾ in their de Haas Shubnikov experiment. Our main interest in this experiment, however, is that it showed that at high fields, the shift in the Fermi level could be quite considerable, and has to be taken into account when one considers the far infra-red cyclotron resonance.⁽⁴³⁻⁴⁴⁾ This resonance is observed in our experiment. This matter is considered in more detail in Chapters II and III. In common with Brown et. al.⁽³⁾ we see no oscillations which can be associated with the hole band.

CHAPTER II

BISMUTH

Our Experiments

There were two essential reasons why we carried out the experimental study discussed in this chapter. First of all, the equipment had been considerably improved* since the experiments of Brown, Mavroides and Lax.⁽⁴⁻⁵⁾ A greater range of magnetic fields and photon energies were available, and the resolution and signal-to-noise ratio had been improved. Secondly, some of the experiments discussed in Chapter I, performed subsequent to the Brown, Mavroides and Lax investigation, had indicated that there might be some additional fine structure in the magnetorefectivity⁽³⁶⁻³⁸⁾ that had not been observed in the original experiments. These two development led us to believe that a careful reinvestigation of the magneto-optical properties of bismuth with the improved appratus might yield some new information.

In Section A of this chapter, we will describe the experimental apparatus, sample preparation techniques, and experimental procedures which were used. In Section B, we will present our data and analyze it in terms of the two band model of Lax.⁽³⁾ In Section C we will consider in detail the effects of the other nearby bands which are neglected in the Lax model, using the calculation of Baraff which includes these effects to lowest order in perturbation theory.⁽³⁹⁾ We find that, to this approximation, there should be no deviations from the Lax model in the magnetoreflexion resonance spectrum. In Section D, we will summarize our conclusions.

* Most of these improvements were made by Mavroides, Kolesar, and Dresselhaus in the course of their subsequent studies of antimony,⁽⁴⁾ graphite,⁽⁵⁾ etc.

SECTION IIA

Experimental Apparatus and Crystal Preparation

Experimental apparatus

To briefly characterize our experiments, we may state that we measure, at various photon energies, the dependence of the reflectivity of a single crystal semimetallic sample on the magnetic field, using the Faraday geometry. In this geometry, the light is reflected at nearby normal incidence from a sample surface which is also normal to the direction of the magnetic field. The sample is generally cooled to temperatures near that of liquid He, and the light used may be either unpolarized, or linearly polarized.

The experimental apparatus is described in more detail by Figure 2. Two light sources were used: a standard Perkin-Elmer 012-2401 SiC Globar source for long wavelength work and a high intensity tungsten lamp (Sylvania Sun Gun) for photon energies above .5 eV. Since the amplitudes of our oscillations are generally only a few percent of the total reflectivity, we require a very stable light source, so that a well regulated DC power supply (Sorenson Nobatron DCR 150-10A) was used to power both the Globar and the tungsten lamp.

Most of the experiments were performed using a Perkin-Elmer Model 112 double pass prism monochromator, with a built-in 13 cps chopper and synchronous detector, but some high resolution work was done using a Perkin-Elmer Model 12G single pass grating monochromator, which lacks such a chopper. A Bulova model 2 MAS42CM 13 cps tuning fork chopper was placed at the output of this instrument.

For some experiments, the light was linearly polarized by placing a AgCl Brewster angle polarizer in the optical path at the point shown. When this was

done, the degree of polarization always exceeded* 90%. For most experiments, however, no polarizer was used because its attenuation adversely affected the signal to noise ratio of the system. When no polarizer is used, we will call the light beam "unpolarized", as is customary. It should be pointed out, however, that due to the polarizing effects of the prisms in our monochromators (even the grating instrument uses a fore-prism), the ratio of the intensities of the two polarizations in our "unpolarized" beam may be as high as two to one. (45)

The optical system focuses the beam from the monochromator onto the sample through a KBr window in the outer dewar wall; then gathers the reflected light and refocuses it on the detector. The sample is mounted in the center of the magnet as shown. The magnet is a water cooled Bitter selenoid capable of achieving field intensities in excess of 100 KG, with a field uniformity over the sample volume of better than 1%. (46)

Two detectors were used in our experiments: a thermocouple for long wavelength work and a PbS photoconductor for energies above .5 eV. Both of these detectors are normally supplied with the Perkin-Elmer model 112 monochromator system. Following the detector is a synchronous amplifier. With the Model 112 prism monochromator, the standard Perkin-Elmer Model 107 amplifier is used, but with the model 12G grating instrument, a Princeton Applied Research Model HR-8 synchronous amplifier is substituted. Following the amplifier is a calibrated buck-off unit which eliminates the large DC voltage corresponding to the zero field reflectivity, so that we may more conveniently observe the small oscillations in which we are interested.

* The depolarization is essentially due to the slight tilt of the polarized beam with respect to sample's crystalline axes, produced by the complicated optical system required to fold the beam into the small magnet bore.

The signal is now reamplified and fed into the Enhancetron (Nuclear Data Model 800) signal averager. This instrument has two functions. First, of all, at the sweep terminals, it provides a repetitive triangular waveform which is fed into the magnet power supply control circuit, so that the current through the magnet is approximately directly proportional to the sweep voltage with a small and somewhat random delay which always seems to be under 1.5 seconds. Secondly, by sequentially sampling, digitalizing, and processing the input signal voltage, the instrument generates and stores an average input voltage vs. sweep voltage curve, which essentially describes the average dependence of the reflectivity on the magnetic field. The average is over any number of sweeps, with the signal to noise ratio increasing as $\sqrt{N}$, where N is the number of sweeps. The great advantage of this system is that it allows us to average out the large amount of low frequency noise in the system which has a period on the same order of magnitude as that of the oscillations in which we are interested. The stored average curve is displayed on the X-Y recorder, while the readout switch is opened to deactivate the magnetic field. The improvement obtained with the Enhancetron is shown in Figure 3, where we show the input to the instrument, as measured by the strip recorder, and the output, as displayed on the X-Y recorder.

The use of the Enhancetron does introduce two new difficulties, however. The first problem has to do with the calibration of the magnetic field. The field vs. current characteristics of the magnets at the NML (Francis Bitter National Magnet Laboratory) are periodically measured to adequate accuracy* by

* This accuracy is about $\pm 1\%$. Most of the uncertainty comes from the long term drift in the field vs. current relation between calibrations. The drift is due to the deformation of the conductors in the magnet under the high magnetic and vibratory loadings produced by fields on the order of 100 kG and cooling water flow rates on the order of 900 gallons per minute.

NML personnel, but unfortunately, the design of the control system makes it inconvenient to continuously monitor the current through the magnet.⁽⁴⁷⁾

Therefore a Hall probe is used to monitor the field, and the Hall probe is calibrated by energizing the magnet with accurately known currents. Since both the Hall probe and the magnet are somewhat nonlinear, many calibration points are needed.

The use of the Enhancetron adds still another step to the calibration procedure, since the X axis of the output curve is proportional to neither field nor Hall probe voltage. Instead, it is proportional to sweep voltage, which is proportional to time, so that one must use the relation between time and Hall probe voltage, recorded on the strip recorder, to complete the calibration.

In spite of all these calibration steps, it is estimated that the field may be determined to better than $\pm 2\%$. The nonlinearities in the calibration curve lead to the nonlinearities in the magnetic field scale displayed in many of our figures.

The second problem stems from the time lag on the order of one second between the sweep voltage and the magnetic field. This displaces the reflectivity curve stored in the Enhancetron while the field is increasing to apparently higher fields; and displaces the curve recorded when the field is decreasing to apparently lower fields. Under standard operating conditions (256 sec. to go from zero to about 100 kG), this corresponds to a total displacement between the two curves of about 1 kG. This introduces little difficulty at high magnetic fields, but at low magnetic fields, where the period of the oscillations is on the order of one kG or less, this displacement can give rise to beat patterns. At the points of constructive interference

one can often see what appears to be small peaks in the reflectivity, and as a matter of fact, some of these spurious peaks were mistakenly reported as real oscillations associated with a new series of interband transitions at the New York, January 1966 meeting of the American Physical Society,⁽⁴⁸⁾ before we became aware of the difficulties associated with the beat patterns.

In summary, we will list the five improvements which have been made in the apparatus since the experiments of Brown, Mavroides and Lax:

- a) The use of a well regulated power supply to increase the source stability;
- b) The use of a grating monochromator to increase the spectral resolution;
- c) The use of the Enhancetron to increase the signal to noise ratio;
- d) The construction of the high field facilities of the NML, which increased the peak fields available; and
- e) Changes in the monochromator system to increase the range of photon energies available, particularly at the low frequency end of the spectrum.

CRYSTAL PREPARATION AND MOUNTING

Bismuth is a soft, silvery material of metallic appearance. Due to its low melting point of 217°C ,⁽⁴⁹⁾ and the absence of any allotropic forms,⁽⁹⁾ it is quite easy to prepare in pure single crystal form. It also cleaves easily and is not particularly reactive, and is, in fact, sometimes found free in single crystal form in nature.⁽⁴⁹⁾ These properties make it an excellent experimental material.

Our samples were made from single crystal boules of bismuth prepared from material of 99.9999% purity, and grown⁽⁵⁰⁾ by pulling from the melt. The boule was cleaved to locate the trigonal axis,⁽⁹⁾ which is perpendicular to the easy cleavage plane, and the binary and bisectrix axes were located from Laue X-Ray

diffraction patterns. The samples were then spark cut,⁽⁵¹⁾ with all faces perpendicular to one of the principal axes. The binary and bisectrix optical faces were spark planed and electropolished,⁽⁵²⁾ but the trigonal faces were left in their as-cleaved condition.

To mount the sample, a very simple procedure has been found to be adequate.⁽⁵³⁾ The dewar is inverted and a slot in the copper block at the end of the cold finger is partially filled with Duco cement. While the cement is drying, the sample is placed into this slot and an alignment jig is fitted to the dewar. This jig shines a beam of light on the optical face of the sample, and when the sample has been oriented so that the reflected beam from the sample strikes a pair of cross hairs, then it has been oriented with its optical face perpendicular to the dewar axis. The jig which holds the dewar in the magnet keeps the dewar axis parallel to the selenoid axis. The magnetic field and the crystalline principal axis perpendicular to the optical face are probably aligned to within two degrees. This conclusion is born out by certain features of the experimental data which will be discussed in the next section.

SECTION IIB

Experimental Results

In this section we will discuss the results of our magnetorefectivity experiments, and analyze the magnetorefectivity spectra we have obtained in terms of the two band model of Lax.⁽³⁾ Since bismuth is a highly anisotropic material, we will find that our experimental results are very strongly dependent on the sample orientation, and we will therefore discuss each sample orientation separately.

BINARY ORIENTATION

In this case, where we have set the magnetic field and the propagation vector of the light parallel to the binary axis, our data are essentially identical with those obtained by Brown, et. al.,⁽³⁾ except that we have made our observations over a more extended range of fields and photon energies, and we have obtained a somewhat better signal-to-noise ratio, due to the improvements that have been made in the equipment since the time of the original experiments. An experimental trace, representative of those observed in the photon energy range from .09 to .2 eV., is shown in Figure 4. These oscillations are due to interband transitions between the tightly coupled valence and conduction bands associated with the electrons, which are described by the two band model of Lax. In particular, these oscillations are associated with the interband transitions which lie near the two nonprincipal L points in the Brillouin zone (see Section IA for definitions.) Oscillations associated with interband transitions lying near the principal L point are not seen, because the corresponding principal ellipsoid has a very large cyclotron effective mass so that these oscillations are unobservably small.

These data also indicate that the sample has been accurately aligned with respect to the magnetic field, since if the field were not very nearly parallel to the binary axis, the effective cyclotron masses for the two non-principal electron ellipsoids would be non-equivalent, so that the observed magneto-reflectivity oscillations would display doublet structure. The lack of any such structure indicates that our sample is aligned with respect to the magnetic field to well within two degrees.

At lower photon energies, the experimental traces look very different from the one we have been discussing. A representative trace measured at a photon energy of .0751 eV is displayed in Figure 5. In this figure, the complicated pattern of the low field, high quantum number oscillations is a spurious effect, due to the delays in the Enhancetron circuits, as discussed in Section IIA. The unusual shape of the $n = 0$ oscillation is real, however. Furthermore, the determination of the energy gap is critically dependent upon a correct interpretation of the lineshape of the $n = 0$ oscillation, since it is the only one that may be experimentally observed at photon energies which are low enough so that the energy gap is at all comparable with the magnetic energy. The lineshape calculation of Chapter III indicates that the critical field (as defined in Section IB) is very close to the reflectivity peak for all the interband transitions, (See Figures 17 and 18), so we have experimentally defined the resonant field as the field at the reflectivity peak, in agreement with the practice of Brown, et. al.

When we plot the resonant fields as a function of photon energy, we obtain the experimental points on the fan chart of Figure 6. To fit the Lax model to these experimental data, we wrote a computer program to minimize the root-mean-squared error between the critical fields predicted by Equations IB8

to 10, and the experimentally measured resonant fields. With

$$\beta^* = .00745 \text{ eV/kG} ,$$

$$m_c = \frac{\hbar |e|}{m_o c} \frac{1}{\beta^*} = \frac{|\vec{m}^*|^{1/2} H}{\{\vec{H} \cdot \vec{m}^* \cdot \vec{H}\}^{1/2}} = .00156 ,$$

and

$$E_g = .011 \text{ eV} ,$$

we obtained the theoretical curves shown as solid lines of Figure 6. At low photon energies, the agreement between theory and experiment is excellent.

At very high photon energies, however, we note that the agreement between the theoretical and experimental points is not so good. In Figure 7, we display a high energy experimental trace where it can be seen that the line shape is also considerably different from what it was in Figure 4. We therefore, conclude that at these highest photon energies, other bands⁽³⁹⁾ are becoming important, and the Lax model is beginning to break down.

In addition to the interband transition oscillations which we have been discussing, the experimental trace of Figure 5 also displays structure which has been associated with an intraband cyclotron resonance transition. In this case, we experimentally define the resonance field as the field at the steepest portion of the cyclotron resonance lineshape, since theory indicates that the critical field will lie close to this value for the range of photon energies observed in our experiments (See Section III F for details.) It should be pointed out, however, that the details of the cyclotron resonance lineshape are not as well understood as the details of the interband transition lineshape, and we will therefore not attempt to extract any band parameters from the

cyclotron resonance data. We have, however, also plotted these resonant fields on the fan chart of Figure 6. From Equations IB8-9 for the Landau level energies, we see that we may easily obtain the corresponding theoretical cyclotron resonance curve, shown dashed on Figure 6, by simply subtracting E_g , the energy gap, from the theoretical curve for the $n=0$ interband transition. Although we have introduced no new adjustable parameters, the agreement between theory and experiment is, once again, quite good.

BISECTRIX ORIENTATION

If one places the magnetic field and the propagation vector of the light perpendicular to the bisectrix face, one obtains more complicated experimental traces than one finds for the binary orientation. Representative experimental traces measured at high and low photon energies are displayed in Figures 8a and 9, respectively. Once again, these oscillations are essentially identical with those observed by Brown, et. al., and are due to interband transitions between the tightly coupled valence and conduction bands associated with the electrons. In this case, however, both the principal and non-principal ellipsoids have small cyclotron effective masses, so that both of the associated series of oscillations are observed. For the bisectrix orientation, the electrons in the two equivalent non-principal ellipsoids are the "heavy" electrons, and the electrons in the single principal ellipsoid are the "light" ones.

We have analyzed this data in precisely the same way as we analyzed the binary data. Defining the experimental resonance conditions for interband and cyclotron resonances as we did before, we have plotted the resonance fields on the fan chart of Figure 10. Fitting the Lax model to the data for the interband transitions, we find:

$$\beta^* = .00844 \text{ eV/kG} ,$$

$$m_c = .00138 ,$$

and

$$E_g = .011 \text{ eV} ,$$

for the light electrons; and

$$\beta^* = .00424 \text{ eV/kG} ,$$

$$m_c = .00273 ,$$

and

$$E_g = .011 \text{ eV} ,$$

for the heavy electrons. Once again, the theoretical interband and cyclotron resonance critical fields, and the experimentally measured resonance fields are in excellent agreement.

All the experimental traces displayed so far were measured using unpolarized light. When polarized light is used for the bisectrix orientation, however, the pronounced effect shown in Figure 8b is observed.⁽²⁷⁾ We see that when the optical electric field is parallel to the binary axis, the oscillations associated with the heavy electrons are almost completely extinguished, though the oscillations associated with the light electrons are large for both polarizations of the optical electric field. This effect is due to the large anisotropy of the electronic effective mass tensors, which causes the bands associated with the various ellipsoids to couple differently to the two polarizations of the optical electric field. (See Chapter III for a detailed description of this coupling.) Similar polarization experiments were carried

out for the binary orientation, and, as expected, no striking effects were observed.

TRIGONAL ORIENTATION

A representative experimental trace for this orientation is shown in Figure 3. Once again, these oscillations are due to interband transitions between the tightly coupled valence and conduction bands associated with the electrons, and described by the two band model of Lax.⁽³⁾ Oscillations for this sample orientation have not been previously observed, however, due to their small amplitude which arises from the fact that the cyclotron effective mass for the electron ellipsoids is relatively large for this direction of magnetic field. All the electron ellipsoids are equivalent for this sample orientation, so that only one series of oscillations is observed.

To analyze the data, we once again experimentally define the resonance field as the field at the peak in the reflectivity (See Figure 19 for the theoretical justification), and plot these fields on the fan chart of Figure 11. In this case, we experimentally observe neither the cyclotron resonance line, nor the $n=0$ interband resonance, because they both occur at very low photon energies. Since we cannot obtain a reliable value for E_g without this data, we have used the value of .011 eV. obtained from the binary and bisectrix data, and then varied β^* to get the optimum root-mean-squared fit to the data. Using this value of

$$\beta^* = .00125 \text{ eV/kG} ,$$

or

$$m_c = .00926 = \frac{\pi |e|}{m_o c} \frac{1}{\beta^*} ,$$

we calculate the solid theoretical curves shown in Figure 11. Once again, the agreement between theory and experiment is excellent.

SECTION IIC

Departures from the Lax Model

So far we have been assuming that the Lax model is precisely correct, and have found that this assumption gives excellent agreement with experiment. Upon more detailed analysis, however, we find that there are several reasons why this excellent agreement is rather surprising. First of all, the essential assumption of the Lax model is that the interaction between the two strongly coupled bands is much greater than the interaction of these two bands with the other bands nearby.⁽²⁷⁾ It would therefore be natural to doubt the validity of this assumption in regions of the Brillouin zone where the band curvature is very small, because this small curvature would indicate that the two "strongly coupled" bands were not strongly coupled at all.⁽⁵⁴⁾ Our data, however, indicates that the Lax model works very well, even in regions of the Brillouin zone where the band curvature, calculated from the Lax model, is so small that it can be described by an effective mass tensor which is much greater than one in all directions.

In order to demonstrate this surprising result, we will consider our interband transitions from the point of view of the semiclassical approximation.⁽⁵⁵⁾ In this approximation, our interband transitions are between orbits in the Brillouin zone, and using the dispersion relations for the Lax model (See Equation IB5) it can be easily shown that these orbits lie in a region of the Brillouin zone where the curvature of the bands is described by the effective mass tensor $\overleftrightarrow{m}(\hbar\omega)$, where

$$\overleftrightarrow{m}(\hbar\omega) = \overleftrightarrow{m}^* \left\{ \frac{\hbar\omega}{E_g} \right\}^3,$$

where $\overleftrightarrow{m}^*$ is the effective mass tensor at the bottom of the band, and $\hbar\omega$ is the

photon energy. Experiments show that the band curvature is highest in the x direction,⁽⁴⁰⁾ where m_{xx}^* has the very small value of .00088 (See Table II). Because of the rapid variation of $\vec{m}(\hbar\omega)$ with $\hbar\omega$, however, one finds that $m_{xx}(\hbar\omega) = 1$ at a photon energy of only .114 eV, though the Lax model still describes the magnetoreflexion data very well at much higher photon energies, where it predicts that $m_{xx}(\hbar\omega)$ is much greater than one.

Secondly, the Lax model predicts that all the Landau levels, except the two closest to the gap, will be doubly degenerate. There is, however, clear experimental evidence that this degeneracy is split at the Fermi level by a considerable amount.⁽³⁶⁻³⁸⁾ The size of these splittings depends on the direction of the magnetic field, but is on the order of 10% of the Fermi energy for fields in the binary-bisectrix plane. Since splittings of this magnitude could have easily been observed in our magnetoreflexivity measurements, it is somewhat surprising that the Lax model provides such an excellent fit to our data. In this section, we will work out the implications of our failure to observe any such splittings in the magnetoreflexivity data. In this way, we will be able to obtain some very useful information about the band structure of bismuth, and be able to understand why the Lax model describes the magnetoreflexivity spectrum so well, even in regions of low band curvature.

First of all, it is reasonable to assume that the departures from the Lax model are due to the existence of a small but significant interaction between: (a) the strongly coupled conduction and valence bands; and (b) the other bands nearby.⁽³⁹⁾ Such an interaction would shift the various Landau levels by unequal amounts, and in this way split the Lax degeneracy. An expression for these energy shifts, which we would like to investigate, can be obtained from the work of Baraff,⁽³⁹⁾ who considered the interaction as a

small perturbation, and calculated these shifts to the lowest order in perturbation theory, with $\hbar k_H$, the crystalline momentum parallel to the magnetic field, set equal to zero.

To describe Baraff's rather complicated results, it is convenient to first define* the quantum number, j , as

$$j = n + \frac{1}{2} - \frac{1}{2} S \quad . \quad (\text{IIC1})$$

We will, hereafter, use the quantum numbers j and S in place of the quantum numbers n and S . We may now write $E_0(j)$, the unperturbed Lax energy, in the simpler form

$$E_0(j) = \pm \sqrt{\frac{E_g^2}{4} + E_g \beta_w^* H j} \quad , \quad (\text{IIC2})$$

where

$$\beta_w^* H = \frac{|e| \hbar}{m_o c} \left\{ \frac{\vec{H} \cdot \overleftrightarrow{m}_w \cdot \vec{H}}{|\overleftrightarrow{m}_w|} \right\}^{1/2} \quad , \quad (\text{IIC3})$$

$\overleftrightarrow{m}_w$ is a tensor to be experimentally determined, and the plus and minus signs refer to the conduction and valence bands, respectively. Equation IIC2 explicitly displays the Lax degeneracy, since $E_0(j)$ does not involve S . One should note, however, that there is no state with $j=0$ and $S=-1$, since this would imply $n=-1$, and therefore the lowest state is nondegenerate.

We may now write the shift in the Landau level energy, $\Delta E(j,S)$, due to the perturbation, as

*Note that we have used the notation of Section IIIE, where these expressions have been rederived, rather than the notation used by Baraff.

$$\begin{aligned}\Delta E(j,S) &= \frac{2E_o(j)+E_g}{4E_o(j)} \{2B_a^c \beta_w^* H_j + H\nu_c S\} \\ &+ \frac{2E_o(j)-E_g}{4E_o(j)} \{2B_a^v \beta_w^* H_j - H\nu_v S\}\end{aligned}\quad (\text{IIC4a})$$

when $E_o(j) \neq -E_g/2$, and

$$\Delta E(0,+1) = H\nu_v \quad (\text{IIC4b})$$

when $E_o(j) = -E_g/2$. In these expressions, we have defined

$$H\nu_i = \frac{\vec{H} \cdot \overset{\leftrightarrow}{F}_i \cdot \vec{H}}{(\vec{H} \cdot \overset{\leftrightarrow}{m}_w \cdot \vec{H})^{1/2}}, \quad (\text{IIC5a})$$

and

$$B_a^i = \frac{\vec{H} \cdot \overset{\leftrightarrow}{D}_i \cdot \vec{H}}{\vec{H} \cdot \overset{\leftrightarrow}{m}_w \cdot \vec{H}}, \quad (\text{IIC5b})$$

where $i = v$ or c , and $\overset{\leftrightarrow}{m}_w$, $\overset{\leftrightarrow}{F}_c$, $\overset{\leftrightarrow}{F}_v$, $\overset{\leftrightarrow}{D}_c$ and $\overset{\leftrightarrow}{D}_v$ are all tensors to be experimentally determined. If they were all truly nonzero and independent, this determination would be a very formidable job. Using the results of our magnetorefectivity experiments, however, the problem can be vastly simplified.

In order to explore the effects of the energy shifts $\Delta E(j,S)$, predicted by Baraff, on the magnetorefectivity spectrum, we will now investigate the properties of the various allowed inter-Landau level transitions. In the Lax model, the selection rule for these transitions⁽¹⁰⁾ is $\Delta j = \pm 1$, $\Delta S = \pm 2, 0$. See Section IIID for details. It is argued in Section IIIE that the small departures from the Lax model considered by Baraff will leave these selection rules essentially unaffected. In Figure 12 we have therefore used these selection

rules to draw eight of the allowed interband transitions which would all be degenerate in the Lax model. If all the additional tensors introduced by Baraff were unrelated, it can be seen that these transitions would all occur at slightly different photon energies.

Of these eight interband transitions, four are spin conserving, and four are not. In Figures 20a and b, we display representative curves for the contributions of both types of transitions to the conductivity as a function of magnetic field, using the theory we have developed in Chapter III. It can be seen that the spin conserving transitions yield large, sharp, resonant peaks in the conductivity, having the same asymmetry as the conductivity curves calculated by Dresselhaus and Dresselhaus.⁽²⁸⁾ The spin flipping transitions, on the other hand, yield smaller, blunter, and more symmetric contributions to the conductivity. In addition, these contributions are "nonresonant" in the sense that their amplitude is essentially determined by the band structure, and is independent of the relaxation time. For these reasons, we find upon actually carrying out the calculations that the oscillations in the reflectivity due to the spin flipping transitions are unobservably small.

Our magnetorefectivity data, therefore, indicates that all the spin conserving interband transitions in Figure 12 are degenerate, for if this were not true, the magnetorefectivity data would display pronounced fine structure. In order for the transitions from the S, j , conduction Landau level to the $S, j+1$, valence Landau level to be degenerate with the transitions from the $S, j+1$, conduction Landau level to the S, j , valence Landau level; we require that

$$-B_a^v = B_a^c \equiv B_a \quad (\text{IIC6a})$$

Furthermore, in order for the transitions from the S, j , conduction Landau level

level to the $S, j+1$, valence Landau level to be degenerate with the transitions from the $-S, j$, conduction Landau level to the $-S, j+1$, valence Landau level; we require that

$$-v_v = v_c \equiv v. \quad (\text{IIC6b})$$

Since no splitting of the peaks in the magnetorefectivity was observed for any orientation of field, it is very likely* that we may also write

$$\overleftrightarrow{\hat{D}}_v = \overleftrightarrow{\hat{D}}_c \equiv \overleftrightarrow{\hat{D}}, \quad (\text{IIC7a})$$

and

$$\overleftrightarrow{\hat{F}}_v = \overleftrightarrow{\hat{F}}_c \equiv \overleftrightarrow{\hat{F}}. \quad (\text{IIC7b})$$

So far we have considered interband transitions which do not involve the $j=0, S=1$, valence Landau level, which has an anomalous energy shift (See Equation IIC4b.) It is found, however, that the interband transitions which do involve this Landau level also have an anomalous lineshape, with the role of the spin flipping and conserving transitions essentially interchanged (See Figures 20c and d.). Therefore, even in this case, the transitions which give rise to the large oscillations in the reflectivity are degenerate, so that one expects to see no splitting in the magnetorefectivity spectrum.

Although there is no simple symmetry argument, which predicts the relationships indicated in Equations IIC7a and b, it seems highly unlikely that these

* Rigorously, the relations we have discussed tell us nothing about the (xz) and (yz) tensor components. However, if these components fail to satisfy Equation IIC7 to a significant degree, this would imply that the constant energy surfaces in the valence band are tilted with respect to the constant energy surfaces in the conduction band. As will be explained in Section IVD, such a tilt leads to a breakdown in the selection rules which we do not observe in our experiment.

relationships are purely accidental. Since the tensors $\hat{F}$ and $\hat{D}$ are determined by expressions which have the form of the f-sum rule (See Chapter III for details), a sufficient (though not necessary) condition for Equations IIC7a and b is that at the L point in the Brillouin zone, there be a peculiar "mirror symmetry" of the energy bands about the center of the energy gap between the strongly interacting valence and conduction bands. More explicitly, the condition is that for every band, with energy E at the L point, which interacts appreciably with the conduction band, there is another band, with energy -E at the L point, which interacts just as strongly with the valence band. It is interesting to note that band structures for bismuth having precisely these features have previously been proposed on the basis of purely theoretical considerations. (13)

In Section IIIE we will use Equations IIC7a and b to greatly simplify the expressions for the total Landau level energy, $E_D(j, S)$ which includes both the Lax energy and the Baraff energy shift; D is the band index which takes the values +1 and -1 for conduction and valence bands, respectively. The expressions we find are (for $\hbar k_H = 0$)

$$E_D(j, S) = DE'_0(j) + S\omega_H \quad (\text{IIC8a})$$

when $E'_0(j) \neq -\frac{E_g}{2}$, and

$$E_{-1}(0, +1) = -\frac{E_g}{2} - \hbar\nu \quad (\text{IIC8b})$$

when $E'_0(j) = -\frac{E_g}{2}$, where we have defined

$$E'_0(j) = \sqrt{E_g^2/4 + E_g \beta^* H_j} \quad , \quad (\text{IIC9a})$$

$$H\beta^* = \frac{|e|\hbar}{m_0 c} \frac{(\vec{H} \cdot \vec{m}^* \cdot \vec{H})^{1/2}}{|\vec{m}^*|^{1/2}} \quad , \quad (\text{IIC9b})$$

and

$$H\nu = \frac{\vec{H} \cdot \vec{F} \cdot \vec{H}}{(\vec{H} \cdot \vec{m}^* \cdot \vec{H})^{1/2}} \quad , \quad (\text{IIC9c})$$

where $\vec{m}^*$ and $\vec{F}$ are tensors to be experimentally determined.* The first term of Equation IIC8 has precisely the form of the Lax equation, and the second term describes the splitting of the Lax degeneracy by the interaction with the nearby bands, to the first order in perturbation theory.

We now can see why the Lax model describes the magnetorefectivity spectrum so well. First of all, the interband transitions which yield large oscillations in the reflectivity, are between Landau levels that are both shifted in the same direction by the second term of Equation IIC8, so that the resonant fields and photon energies are unaffected. Secondly, the strongly resonant intraband transitions are spin conserving ones (See Figures 20e and f), so that these also yield oscillations with resonances which are also described by the Lax model. Therefore, the energy gap, E_g , and the tensor, $\vec{m}^*$, which appear in Equation IIC8, are precisely the ones we have measured in our experiments, and only the tensor $\vec{F}$ remains to be determined. It can be shown that $\vec{F}$ has the same form as $\vec{m}^*$, so that for the principal ellipsoid

* Note that $\vec{m}^*$ is a combination of $\vec{m}_w$ and $\vec{D}$, but we need not determine these two tensors separately.

$$\vec{F} = \begin{pmatrix} \vec{F}_1 & 0 & 0 \\ 0 & \vec{F}_2 & \vec{F}_4 \\ 0 & \vec{F}_4 & \vec{F}_3 \end{pmatrix}, \quad (\text{IIC10})$$

and only four independent parameters remain to be found. These parameters could be measured by determining the Landau level splitting at the Fermi level as a function of field orientation by a DHVA type experiment.⁽³⁶⁻³⁸⁾ Once this has been done the effects of the Baraff interaction on the Landau level structure, up to the first order in perturbation theory, can be completely taken into account by using Equations IIC8 and 9.

To summarize our results, we have found an expression for the energies of the Landau levels^{*} associated with the tightly coupled valence and conduction bands at the L points in bismuth, which includes the Baraff interaction to the first order in perturbation theory. This expression predicts that the Lax degeneracy may be split by a considerable amount, while the magnetorefectivity spectrum is still adequately described by the Lax model. It should be noted, however, that in order to understand the magnetorefectivity lineshape, the Baraff interaction must be taken into account. This matter is discussed in detail in Chapter III.

* So far we have only given expressions valid at $k_H = 0$. We have worked out the more general expressions, valid when $k_H \neq 0$, in Section IIIE.

SECTION IID

Discussion of Results

In this Section we will compare our results with the band parameters reported by some other experimentalists^(3,37) (See Table I.) We will also suggest some additional experiments which might yield useful results. Before discussing Table I, however, we will make a few comments about the parameters of Smith, Baraff, and Rowell⁽³⁷⁾ (SBR). In their experiments, they measured the DHS oscillations in the resistivity of bismuth, taking into account the variation of the Fermi level with the magnetic field. The interpretation of such an experiment requires the determination of a great many parameters, and so they obtained many of them from a careful study of the literature. In particular, the value they quote for E_g was taken from the previous magneto-reflection experiments of Brown, Mavroides and Lax⁽³⁾ (BML), and therefore does not represent an independent evaluation of this parameter.

As a matter of fact, upon a careful search of the literature, we have not been able to find any other reasonably accurate and direct determination of E_g . Therefore, the only determination of E_g available for comparison with our own is the previous determination by BML. In Table I, however, we note that there is a large discrepancy between these two values. The reason for this discrepancy probably is the very small size of E_g , which is much less than the kinetic energy of the electrons, even at the Fermi energy. As a result of its small magnitude, E_g is rather hard to measure, even by an infra-red magneto-optical experiment, and extreme accuracy in the experimental measurements of the resonance fields and photon energies is necessary. Therefore, due to the improvements that have been made in the equipment since the time of the original experiments, we conclude that our value of $E_g = .011$ eV

represents a refinement on the value of $E_g = .015$ eV measured by Brown, Mavroides and Lax.

It will next be noted from Table I that our values for β^* also disagree with the values measured by BML and SBR. These differences, however, are essentially due to the different values we have used for E_g . The reason why the choice of E_g affects the determination of β^* can be understood by referring to Equation IB8a. We see from this equation that when the Landau level energy, E , is considerably greater than E_g , we can approximate E by the equation

$$E = \left\{ \frac{E_g}{2} (\beta^* H [2n+1-S] + \frac{\hbar^2 k_H^2}{m_o m_H}) \right\}^{1/2} \quad (\text{IID1})$$

This approximation is reasonably valid even at the Fermi level, so that the three experiments under discussion all essentially measure $E_g \beta^*$ rather than β^* alone. If we therefore compare our values of $E_g \beta^*$ to the values determined by other experimentalists, we see that the agreement is much better. The agreement with the values given by SBR, in particular, is quite good. Since these values were obtained after a careful search of the literature for the most accurate values available, we conclude that our measurements are in good agreement with those obtained by other experimentalists.

In order to completely determine the Landau level energies at $k_H = 0$, we would now like to determine the tensor $\hat{F}$. This tensor could be obtained by fitting Equations IIC8 and 9 to an experiment which measured the Landau level splitting at the Fermi surface. Such experiments were carried out by SBR and other experimentalists, who, however, fit their data to an expression of the form

$$E = \sqrt{\frac{E_g^2}{4} + \frac{E_g}{2} \beta^* H(2n+1-\gamma S)} \quad , \quad (\text{IID2})$$

where E is the Landau level energy at $k_H = 0$, and γ is a number slightly different from unity. In particular, SBR, whose data are very complete, assumed that the transformation properties of the quantity $\beta^*(1-\gamma)$ were described by the relation

$$H\beta^*(1-\gamma) = \frac{|e|\hbar}{m_o c} \left\{ \frac{(\vec{H} \cdot \vec{m}^* \cdot \vec{H})^{1/2}}{|\vec{m}^*|^{1/2}} - \frac{(\vec{H} \cdot \vec{m}_S^* \cdot \vec{H})^{1/2}}{|\vec{m}_S^*|^{1/2}} \right\} \quad , \quad (\text{IID3})$$

where $\vec{m}^*$ and $\vec{m}_S^*$ are tensors to be experimentally determined.

It is important to emphasize that Equations IID2 and 3 have no firm theoretical basis. They are, however, able to give at least a qualitative fit to the DHS data of SBR, though they appear to have a very different form than Equations IIC8 and 9. We will, therefore, see whether or not we can put Equations IID2 and 3 in a form similar to the form of Equations IIC8 and 9. To do this, we first consider $1-\gamma$ a small perturbation, and expand the square root in Equation IID2 to find

$$E = E'_o(j) + \frac{(1-\gamma)\beta^* E_g}{4E'_o(j)} SH \quad , \quad (\text{IID4})$$

using the notation of Equations IIC8 and 9. The expressions of SBR therefore predict that the conduction band Landau levels are split with an effective splitting parameter, v^* , of

$$v^* = \frac{(1-\gamma)\beta^* E_g}{4E'_o(j)} \quad . \quad (\text{IID5})$$

Assuming that $1-\gamma$ is much less than unity, we may also define

$$\hat{d} \equiv \frac{\vec{m} \cdot \vec{m}_S}{|\vec{m}| |\vec{m}_S|} \quad (\text{IID6})$$

and then expand the square roots in Equation IID3 to obtain

$$H\nu^* = \frac{|e|\hbar E_g}{8m_0 c E'_0(j) |\vec{m}|^{1/2}} \frac{\vec{H} \cdot \vec{d} \cdot \vec{H}}{(\vec{H} \cdot \vec{m} \cdot \vec{H})^{1/2}} \quad (\text{IID7})$$

Upon comparing Equations IID7 and IIC9, we see that to this order of approximation, the transformation properties of ν and ν^* are the same. The energy dependence of ν^* is, however, incorrect. We therefore conclude that the treatment of SBR is in essential agreement with ours only if E_f can be assumed to be constant. In the experiments of SBR, however, the variations in the Fermi energy were found to be as great as 30%. Therefore we conclude that the analysis of SBR is probably roughly correct, but that a re-analysis of their data, using Equations IIC8 and 9 might yield a noticeable improvement in the agreement between theory and experiment. Actually carrying out this re-analysis is a rather extensive undertaking which we have not attempted. Instead we have merely used Equation IID5 to determine ν^* , using the SBR parameters with $E'_0(j)$ equal to the zero field Fermi energy, and have listed these values of ν^* in Table II. It would, however, be very interesting to do the more extensive calculation, and in this way, obtain an experimental evaluation of the tensor $\hat{F}$.

It would also be interesting to investigate further the peculiar lineshape of the oscillations in the magnetorefectivity at high photon energies (See Section IIB.) Such an investigation might yield further information about the interaction of the two strongly coupled bands with the other bands nearby. These ideas are currently under investigation by Dr. S. Iwasa of the M.I.T.

Physics Department, who is using high resolution laser spectroscopy⁽⁵⁶⁾ to explore these effects in very great detail.

CHAPTER III

THE MAGNETOREFLECTIVITY OF BISMUTH - THEORY

In bismuth, at the magnetic fields and photon energies where interband transition oscillations are observable, the magnetoplasma edge, the cyclotron resonance line, and the $n=0$ interband transition are all nearly degenerate in photon energy.⁽³⁾ Therefore, one requires a very detailed calculation of the magnetorefectivity in order to understand the lineshape of the oscillations in this experimental region. One is particularly interested in this lineshape because the determination of the energy gap is critically dependent upon the proper interpretation of the $n=0$ line. We were also interested in seeing if we could explain the complicated lineshape in the vicinity of the $n=0$ and the cyclotron resonance lines in terms of the two-band model of Lax,⁽³⁾ which explains the magnetoreflexion spectrum so well.

The approach we have used in calculating the magnetorefectivity is to first find the frequency dependent, magnetic field dependent conductivity tensor, σ_{ij} , and to then find the infrared properties of the material using conventional electromagnetic theory.⁽²⁸⁾ The conductivity tensor will be found by calculating the current density, $\vec{J}(t) = \vec{J}e^{-i\omega t}$, which flows for an applied electric field, $\vec{\epsilon}(t) = \vec{\epsilon}e^{-i\omega t}$, as the thermal average⁽²⁸⁾ of the quantum mechanical operator $e\vec{v}$, which is found by taking the trace

$$\vec{J}(t) = \text{Tr}\{e\vec{v}\rho(t)\} \quad ,$$

where e is the charge and $\vec{v}$ is the velocity operator for the particles, and $\rho(t)$ is the time dependent density operator. In using this approach we have implicitly assumed that magnetic dipole coupling, many body, and nonlocal

effects* are negligible, and the effects due to the quantization of the electromagnetic field may be ignored. The major novelty of our approach lies in the consistent way we consider nonparabolic effects in our conductivity calculation, including the $\vec{k}$ dependent velocity matrix element of Wolff.⁽¹⁰⁾

Using the Lax model to describe the tightly coupled conduction and valence bands,^(25,35) we find that the theoretical lineshapes for oscillations associated with interband transitions are in reasonable agreement with experiment, even for the strangely shaped $n=0$ oscillation. We further conclude that the critical field, as defined in Chapter I, closely corresponds to the field at the peak in the reflectivity for all of the interband resonances. Unfortunately, however, only qualitative agreement could be obtained between the theoretical and experimental cyclotron resonance lineshapes.

We therefore went on to consider the small deviations from the Lax model, first treated by Baraff.⁽³⁹⁾ Using Baraff's results, the results of our magnetoreflexion experiments, and the lineshapes predicted by the simple Lax model for the $n \neq 0$ oscillations, where reasonable agreement between theory and experiment had been obtained, we were able to greatly simplify the equations of Baraff, and extend them to the $k_H \neq 0$ case. This is probably the most

*The essential requirement for local conditions at infrared frequencies where $\omega\tau \gg 1$, is that the states which contribute strongly to the material conductivity have average velocities such that they move much less than one wavelength of light during one cycle of the optical electric field.⁽⁵⁹⁾

For intraband transitions, the velocity of interest is clearly the velocity at the Fermi level. For interband transitions, it is not quite so clear what we should use for a characteristic velocity. In the Lax model, however, the bands have a linear dependence on the crystalline momentum for large values of $\hbar\vec{k}$, which implies a limiting velocity for the corresponding states. Using this velocity, we find that local conditions should apply.

useful result obtained in the entire chapter. In terms of this more accurate theory, we were able to understand both the measured magnetoreflexivity spectrum, which is in excellent agreement with the Lax model, and the observed spin splitting of the Landau levels at the Fermi surface,⁽³⁶⁻³⁸⁾ which is in disagreement with the predictions of the Lax model.

Due to the complexity of this more accurate model, we were not able to use it directly to calculate the magnetoreflexion lineshape. We were able to show, however, that the use of the more accurate model would probably reduce most of the discrepancies between the experimental lineshapes, and the theoretical ones calculated from the Lax model. There is one discrepancy, however, which we will show cannot be explained on the basis of any band model whatever. Although we have found no satisfactory explanation for this discrepancy, it only occurs at very low photon energy, and does not interfere with the generally reasonable agreement between theory and experiment for the interband resonances.

We will begin the detailed discussion of our conductivity calculation in Section A of this chapter, where we will introduce the time dependent density operator.^(58,60) Since the band energies and velocity matrix elements will be calculated using the effective mass approximation,⁽⁶¹⁻⁶³⁾ we will discuss the approximation in Section B. In Section C, we will apply the effective mass approximation to calculate the conductivity due to the holes, using a somewhat unusual method of procedure. Although our results are in agreement with the standard expressions,⁽⁶⁵⁾ they are algebraically much simpler, and display the field dependence of the conductivity in an unusually transparent form. Using a similar procedure, in Section D we will calculate the conductivity due to the electrons, using the two band model of Lax.⁽¹⁰⁾ In Section E, we will

consider the effects produced by the terms assumed to be zero in the Lax model, and treated more completely by Baraff.⁽³⁹⁾ Using our magnetorefectivity data, we will be able to greatly simplify and extend these results, and will write simple expressions for the energies of the Landau levels which are more accurate than those given by the two band model of Lax. Finally, in Section F we will discuss some of the features of the theoretical results and the validity of some of the approximations.

SECTION IIIA

Density Operator Technique

In this section we will discuss the use of the time dependent density operator, $\rho(t)$, to calculate the conductivity of a system. Most of the ideas presented here have been extensively discussed in the literature. (58,60,28)

The time variation of the density operator, $\rho(t)$, arises from the time dependence of the total Hamiltonian for the system, $H(t)$; we will assume that $H(t)$ can be written

$$H(t) = H_0 + H'(t) \quad , \quad (\text{IIIA1})$$

where H_0 is a time independent Hamiltonian and $H'(t)$ is a time dependent perturbation.

Let us first consider the simpler problem of finding the density matrix for a time independent system with Hamiltonian $\bar{H}(t)$ where t is some parameter of the Hamiltonian different from time. The Schroedinger equation for such a system is

$$\bar{H}(t)\psi(t,u) = -i\hbar \frac{\partial}{\partial u} \psi(t,u) \quad , \quad (\text{IIIA2})$$

in which the time variable is denoted by u . The reason for this notation will be discussed later on. The γ th eigenvalue, $E_\gamma(t)$, and eigenfunction, $\psi_\gamma(t)$, for this system are solutions of the equation,

$$\bar{H}(t)\psi_\gamma(t) = E_\gamma(t)\psi_\gamma(t) \quad , \quad (\text{IIIA3})$$

and the matrix representation of the density operator for this system, $\rho_0(t)$, is the thermal equilibrium distribution

$$\rho_{0\gamma\nu}(t) = \delta_{\gamma\nu} f[E_\gamma(t)] \quad , \quad (\text{IIIA4})$$

where $f(E)$ is the Fermi function, and the basis $\psi_Y(t)$ is the set of eigenfunctions of the Hamiltonian $\bar{H}(t)$.

Let us now consider a system which changes with time at such a slow rate that it is always in thermal equilibrium. In this case, the system may be treated as an essentially time independent one, with the time, t , appearing as a parameter in the Hamiltonian. We can then set $\bar{H}(t)$ equal to the total time dependent system Hamiltonian, $H(t)$, and use Equations (IIIA3) and (IIIA4) to calculate $\rho_0(t)$, which will then be equal to the total time dependent density matrix, $\rho(t)$, for this system.

In our case, the system changes too quickly for this assumption to be true, so one must write

$$\rho(t) = \rho_0(t) + \Delta\rho(t) \quad , \quad (\text{IIIA5})$$

where $\rho_0(t)$ is the thermal equilibrium distribution evaluated as before and $\Delta\rho(t)$ is the correction term.

To find $\rho(t)$ and $\Delta\rho(t)$ we must consider the exact equation of motion for the density matrix,

$$\frac{\partial \rho(t)}{\partial t} = \frac{i}{\hbar} [\rho(t), H(t) + H_{\text{coll}}(t)] \quad , \quad (\text{IIIA6})$$

where $H_{\text{coll}}(t)$ describes the perturbations in the Hamiltonian produced by impurities, phonons, and all other scattering phenomena. To handle this term we will make the same approximation as one makes in the Boltzmann equation, and assume that the total effect of all the scattering processes is to make this system relax towards thermal equilibrium with a relaxation time τ .

Therefore, one may write

$$\frac{\partial \rho(t)}{\partial t} = \frac{i}{\hbar} [\rho(t), H(t)] + \frac{\rho_o(t) - \rho(t)}{\tau} \quad . \quad (\text{IIIA7})$$

Since we may rewrite Equation IIIA4 in the form of the operator equation

$$\rho_o(t) = f(\bar{H}(t)) = (1 + \exp\{(\bar{H}(t) - E_f)/KT\})^{-1} \quad , \quad (\text{IIIA8})$$

where T is the temperature, K is Boltzmann's constant, and E_f is the Fermi energy; and since any function of an operator commutes with the operator, one may write Equation IIIA7 as⁽⁵⁸⁾

$$\begin{aligned} \frac{\partial \rho_o(t)}{\partial t} + \frac{\partial \Delta \rho(t)}{\partial t} + \frac{\Delta \rho(t)}{\tau} &= \frac{i}{\hbar} [\Delta \rho(t), H_o] \\ &+ \frac{i}{\hbar} [\Delta \rho(t), H'(t)] \quad . \end{aligned} \quad (\text{IIIA9})$$

The second term on the right-hand side is of second order in smallness and is discarded. The remainder of the calculations will be based on this equation.

It will be more convenient to use for our basis throughout the rest of this calculation, the eigenfunctions of H_o , the time independent unperturbed Hamiltonian, rather than those of $\bar{H}(t)$. We can use perturbation theory to expand the eigenfunctions of $\bar{H}(t)$ in terms of the eigenfunctions of H_o and will find

$$\rho_{o_{ij}}(t) = \begin{cases} f(E_j) + \langle \psi_j | H(t) | \psi_j \rangle & \text{if } i=j \\ \frac{\langle \psi_i | H'(t) | \psi_j \rangle}{E_i - E_j} [f(E_i) - f(E_j)] & \text{if } i \neq j \end{cases} \quad , \quad (\text{IIIA10})$$

where E_j and ψ_j are the eigenvalues and eigenfunctions of H_o . One may therefore write a simple equation for the matrix elements of $\Delta \rho(t)$ in terms of those for $\rho_o(t)$

$$\frac{\partial}{\partial t} \Delta \rho_{ij}(t) + \Delta \rho_{ij}(t) \left[\frac{1}{\tau} + \frac{i}{\hbar} (E_i - E_j) \right] = - \frac{\partial}{\partial t} \rho_{o_{ij}}(t) , \quad (\text{IIIA11})$$

where from Equation IIIA10 the time derivative of $\rho_{o_{ij}}(t)$ is simply⁽⁵⁸⁾

$$\frac{\partial}{\partial t} \rho_{o_{ij}}(t) = \begin{cases} \left. \frac{df(E)}{dE} \right|_{E=E_j} \frac{\partial}{\partial t} \langle \psi_j | H'(t) | \psi_j \rangle & \text{if } i=j \\ \frac{f(E_i) - f(E_j)}{E_i - E_j} \frac{\partial}{\partial t} \langle \psi_i | H'(t) | \psi_j \rangle & \text{if } i \neq j \end{cases} . \quad (\text{IIIA12})$$

If the Fermi function for the state with energy E_j is written as $f_j \equiv f(E_j)$ we may finally write for $\Delta \rho_{ij}(t)$

$$\begin{aligned} & \left[\frac{\partial}{\partial t} + \frac{1}{\tau} + \frac{i}{\hbar} (E_i - E_j) \right] \Delta \rho_{ij}(t) \\ &= - \frac{f_i - f_j}{E_i - E_j} \frac{\partial}{\partial t} \langle \psi_i | H'(t) | \psi_j \rangle , \end{aligned} \quad (\text{IIIA13})$$

with the understanding that when $i=j$, $\partial f(E)/\partial E$ is to be substituted for $(f_i - f_j)/(E_i - E_j)$.

We will now discuss the form of the operators H_0 and $H'(t)$ suitable for this conductivity calculation. Assume we know the time independent Hamiltonian for the system with no applied potentials, which we write as $H(\vec{p})$ to emphasize its momentum dependence. We include the applied potentials by replacing $\vec{p}$ by $\vec{p} - \frac{e}{c} [\vec{A}_0 + \vec{A}_{rf}(t)]$, where $\vec{A}_0$ is a time independent vector potential which describes the applied magnetic field and

$$\vec{A}_{rf}(t) = -\frac{ic\hat{\epsilon}}{\omega} \exp\{-i\omega t\} , \quad (\text{IIIA14})$$

where

$$\vec{\epsilon}(t) \equiv \vec{\epsilon} \exp\{-i\omega t\} \quad (\text{IIIA15})$$

is the applied electric field.

This Hamiltonian can be simply Taylor expanded, since $\vec{A}_{rf}(t)$ commutes with the operators $\vec{p}$ and $\vec{r}$, to get the expression

$$\begin{aligned} H[\vec{p} - \frac{e\vec{A}_{rf}(t)}{c} - \frac{e}{c}\vec{A}_0] &= H[\vec{p} - \frac{e}{c}\vec{A}_0] - \frac{e}{c}\vec{A}_{rf}(t) \cdot \vec{v} \\ &+ \mathcal{O}\{[-\frac{e}{c}\vec{A}_{rf}(t)]^2\} , \end{aligned} \quad (\text{IIIA16})$$

where the velocity operator $\vec{v}$ has been written for

$$\vec{v} = \left. \frac{\partial}{\partial \vec{\pi}} H(\vec{\pi}) \right|_{\vec{\pi} = \vec{p} - \frac{e\vec{A}_0}{c}} . \quad (\text{IIIA17})$$

Since we are only interested in the linear response of the system to the field, we only keep the first two terms and make the identifications

$$H_0 = H(\vec{p} - \frac{e}{c}\vec{A}_0) \quad (\text{IIIA18})$$

and

$$H'(t) = \vec{v} \cdot \frac{ie\hat{\epsilon}}{\omega} e^{-i\omega t} , \quad (\text{IIIA19})$$

where H_0 is the unperturbed Hamiltonian. If there is no magnetic field, $\vec{A}_0$ will merely be set equal to zero.

We seek the time variation of the distribution function at the frequency of the electromagnetic perturbation. Therefore, we define $\bar{\rho}$, the amplitude

of the correction term, by the relation

$$\Delta\rho(t) = \bar{\rho} e^{-i\omega t} \quad . \quad (\text{IIIA20})$$

We can now rewrite Eq. IIIA13 as⁽⁵⁸⁾

$$[-i\omega + \frac{1}{\tau} + \frac{i}{\hbar} (E_i - E_j)] \bar{\rho}_{ij} = -e \frac{f_i - f_j}{E_i - E_j} \langle \psi_i | \vec{v} | \psi_j \rangle \cdot \vec{\hat{e}} \quad . \quad (\text{IIIA21})$$

We have now completely evaluated the density matrix. To use the density matrix to evaluate the current, one employs the theorem that the thermal average of any operator, $\mathcal{O}$, is given by the relation⁽⁵⁸⁾

$$\langle \overline{\mathcal{O}} \rangle = \text{Tr}\{\mathcal{O} \bar{\rho}(t)\} \quad . \quad (\text{IIIA22})$$

Thus, the current density, defined as the thermal average of the current density operator is

$$\vec{J}(t) = \vec{J} e^{-i\omega t} = \text{Tr}\{\vec{e} v \bar{\rho}(t)\} \quad . \quad (\text{IIIA23})$$

One can now show that if one treats the applied electric field by introducing a time dependent vector potential, as was done here, the thermal equilibrium distribution, $\rho_0(t)$, makes no contribution to the current at frequency ω . This is because $\rho_0(t)$ was defined as being the thermal equilibrium distribution for the time independent system described by the time independent Hamiltonian $\bar{H}(t)$, where the relationship between $\bar{H}(t)$ and $H(t)$, the total time dependent system Hamiltonian, was discussed near the beginning of this section. Since $\bar{H}(t)$ is time independent, it contains only a constant vector potential and no electric field. Therefore $\rho_0(t)$ contributes no current at frequency ω .

Substituting for $\Delta\rho(t)$ the results of Eq. IIIA20, 21 and 23, we find

$$\vec{J} = - \sum_{i,j} \frac{(f_i - f_j) e^2 \langle \psi_j | \vec{v} | \psi_i \rangle \langle \psi_i | \vec{v} | \psi_j \rangle \cdot \vec{\epsilon}}{(E_i - E_j) (-i\omega + \frac{1}{\tau} + \frac{i}{\hbar} [E_i - E_j])}, \quad (\text{IIIA24})$$

or⁽⁶⁰⁾

$$\sigma_{\alpha\beta} = - \sum_{i,j} \frac{(f_i - f_j) e^2 \langle \psi_j | v_\alpha | \psi_i \rangle \langle \psi_i | v_\beta | \psi_j \rangle}{(E_i - E_j) (-i\omega + \frac{1}{\tau} + \frac{i}{\hbar} [E_i - E_j])}. \quad (\text{IIIA25})$$

In the above relations, the sum is over all of the states. We need only explicitly evaluate the sum, however, for intraband transitions involving bands which contain carriers, and interband transitions between bands for which the energy gap is on the order of, or is less than, the photon energy. The remaining transitions are interband transitions between bands separated by large energy gaps, and we may evaluate their contribution to the conductivity tensor, which we will call the electronic core conductivity, $\sigma_{\alpha\beta}^{ec}$, by first writing

$$\begin{aligned} \sigma_{\alpha\beta}^{ec} &= - \frac{1}{2} e^2 \sum_{i,j} \frac{f_i - f_j}{E_i - E_j} \left\{ \frac{\langle \psi_j | v_\alpha | \psi_i \rangle \langle \psi_i | v_\beta | \psi_j \rangle}{-i\omega + \frac{1}{\tau} + \frac{i}{\hbar} [E_i - E_j]} + \frac{\langle \psi_i | v_\alpha | \psi_j \rangle \langle \psi_j | v_\beta | \psi_i \rangle}{-i\omega + \frac{1}{\tau} + \frac{i}{\hbar} [E_j - E_i]} \right\} \\ &= - \frac{1}{2} e^2 \sum_{i,j} \frac{f_i - f_j}{E_i - E_j} \frac{T_{\alpha\beta}^+ (-i\omega + 1/\tau) + i/\hbar (E_i - E_j) T_{\alpha\beta}^-}{[(-i\omega + 1/\tau)^2 + (E_i - E_j)^2/\hbar^2]}, \quad (\text{IIIA26}) \end{aligned}$$

where the sum is over the large energy gap transitions, and the symmetric and antisymmetric tensors, $T_{\alpha\beta}^+$ and $T_{\alpha\beta}^-$, are given by the relations

$$T_{\alpha\beta}^\pm = \langle \psi_j | v_\alpha | \psi_i \rangle \langle \psi_i | v_\beta | \psi_j \rangle \pm \langle \psi_j | v_\beta | \psi_i \rangle \langle \psi_i | v_\alpha | \psi_j \rangle. \quad (\text{IIIA27})$$

Next we note that when the magnetic field is equal to zero, the conductivity tensor must have no antisymmetric component due to $\vec{T}^-$. This is not true if there is a magnetic field, but in that case, the antisymmetric component will be negligibly small, provided that the energy gaps are much greater than the magnetic energy, as is true for the transitions we are considering in σ^{ec} . Therefore, we may set the second term in Eq. IIA26 equal to zero, whether or not $H=0$, and write

$$\sigma_{\alpha\beta}^{ec} = -\frac{1}{2} e^2 \sum_{i,j} \frac{f_i - f_j}{E_i - E_j} \frac{T_{\alpha\beta}^{+n^2}}{(E_i - E_j)^2} (-i\omega) \equiv -i\omega \epsilon_{\alpha\beta}^{ec}, \quad (\text{IIIA28})$$

which defines the purely real quantity, ϵ^{ec} , the electronic core dielectric constant. Here we have made the approximations

$$(E_i - E_j)^2 \gg |-i\omega\hbar + \hbar/\tau|^2, \quad (\text{IIIA29a})$$

and

$$\omega\tau \gg 1, \quad (\text{IIIA29b})$$

which are valid for the transitions we consider in σ^{ec} . Therefore, we conclude that this contribution to the conductivity tensor may be included in the core dielectric constant, ϵ_c , which is an experimentally determined quantity which also takes into account the polarization of the lattice, and the polarizability of free space.⁽²⁸⁾ It is assumed to be frequency and field independent over the range of photon energies and fields considered in this calculation.

We still must explicitly evaluate the sum of Eq. IIIA25 to evaluate the contributions to the conductivity from both the holes and electrons in both the presence and absence of a magnetic field. To do this, one need find

only the appropriate eigenvalues of the unperturbed Hamiltonian, H_0 and the matrix elements of the velocity operator, evaluated between the eigenfunctions of H_0 . In fact, however, one does not know H_0 or its eigenfunctions, but merely the band parameters of a suitable band model in the effective mass approximation. The use of this information to find the necessary quantities is discussed in the next section.

SECTION IIIB

THE EFFECTIVE MASS APPROXIMATION

For an electron in a solid, one normally knows neither the periodic potential $V(\vec{r})$ in the ordinary one electron Hamiltonian⁽¹⁰⁾

$$H_0 = \frac{p^2}{2m_0} + V(\vec{r}) + \frac{\hbar^2 \nabla^2}{2(m_0 c)^2} V(\vec{r}) + \frac{\hbar^2 \vec{p}}{2(m_0 c)^2} \cdot \vec{s} \times \vec{\nabla} V(\vec{r}), \quad (\text{IIIB1})$$

nor its eigenfunctions and eigenvalues. However, in bismuth the most important part of the infrared conductivity arises from those states corresponding to the solution of H_0 with energies in the vicinity of the Fermi level, and crystal momenta in the vicinity of some high symmetry point in the Brillouin zone.⁽⁶⁶⁾ If we can assume that these states lie in a nearly degenerate subset (NDS) of bands which are coupled to each other much more strongly than they are to any band outside of the NDS, we can then use the effective mass approximation^(61-63,10) to develop a model which accurately describes, in the vicinity of the high symmetry point, both the behavior of the bands in the NDS and the matrix elements of the velocity operator⁽¹⁰⁾ taken between these bands. This energy band model will contain a small number of band parameters which can be determined by experiment.

Since the effective mass approximation has been extensively discussed in the literature,^(10, 61-63) only some of the main features of the technique will be presented here. For simplicity, we will first consider the system in the absence of an external magnetic field. To generate the approximation, it is assumed that the one electron Hamiltonian, H_0 , has been solved to yield the eigenvalues and eigenfunctions for some value of the crystal-line momentum, $\vec{K}_0$, and a suitable nearly degenerate subset of states has been found. For the remainder of this section, quantities indexed by

Roman letters will always be associated with the NDS, while quantities indexed by Greek letters will always be associated with the remaining bands.

If the sets of solutions at $\vec{K}_0$ are u_ℓ and u_ν , with corresponding energies ϵ_ℓ and ϵ_ν , one may use Bloch's theorem and write $\psi_{\vec{k}}^j(\vec{r})$, a solution to the one electron Hamiltonian in the vicinity of $\vec{K}_0$, a distance $\vec{k}$ from $\vec{K}_0$, as

$$\psi_{\vec{k}}^j(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} \phi_{\vec{k}}^j(\vec{r}), \quad (\text{IIIB2})$$

where

$$\phi_{\vec{k}}^j(\vec{r}) = \sum_{\ell=1}^N a_{\ell}^j(\vec{k}) u_{\ell} + \sum_{\nu} a_{\nu}^j(\vec{k}) u_{\nu}, \quad (\text{IIIB3})$$

where $a_{\ell}^j(\vec{k})$ and $a_{\nu}^j(\vec{k})$ are sets of expansion coefficients, and N is the number of states in the NDS. The function $\phi_{\vec{k}}^j(\vec{r})$ is a solution of the equation

$$H \phi_{\vec{k}}^j(\vec{r}) = E_j(\vec{k}) \phi_{\vec{k}}^j(\vec{r}), \quad (\text{IIIB4})$$

where the Hamiltonian H is related to H_0 by

$$\begin{aligned} H &= \frac{(\hbar\vec{k}+\vec{p})^2}{2m_0} + V(\vec{r}) + \frac{\hbar^2 \nabla^2}{8(m_0 c)^2} V(\vec{r}) + \frac{\hbar^2}{2(m_0 c)^2} (\hbar\vec{k}+\vec{p}) \cdot \vec{s} \times \vec{\nabla} V(\vec{r}) \\ &= H_0 + \frac{\hbar^2 k^2}{2m_0} + \vec{v} \cdot \hbar\vec{k}; \end{aligned} \quad (\text{IIIB5})$$

$$\vec{v} = \frac{\vec{p}}{m} + \frac{\hbar^2}{2(m_0 c)^2} \vec{s} \times \vec{\nabla} V(\vec{r}) \quad (\text{IIIB6})$$

is the velocity operator, and $E_j(\vec{k})$ is the energy of band j at a distance $\vec{k}$ from $\vec{K}_0$. Note that the operator $\vec{v}$ includes the effects of spin-orbit coupling.

So far, one has merely rewritten the problem of an electron in a periodic potential without introducing any new approximation. One now makes the two basic assumptions that: (a) the bands in the NDS are much more strongly coupled to each other than they are to any of the remaining bands, and (b) the energy separation between the bands in the NDS is much less than the energy separation between any band in the NDS and any band outside of it.

One can then use perturbation theory to find the expansion coefficients $a_v^j(\vec{k})$, in terms of the coefficients in the NDS, by the relation

$$a_v^j(\vec{k}) = \sum_{\ell} \frac{\langle u_v | \vec{v} | u_{\ell} \rangle \cdot \hbar \vec{k} a_{\ell}^j(\vec{k})}{-\epsilon_v}. \quad (\text{IIIB7})$$

In deriving this relation we have approximated $E_j(\vec{k}) - \epsilon_v$ by $-\epsilon_v$, thereby setting the energy zero at the center of the NDS. The effective mass approximation is valid only if all the $a_v^j(\vec{k})$ are small.

Using this relation, one may derive from equations IIIB4 and IIIB5 a matrix eigenvalue problem which only involves the coefficients $a_{\ell}^j(\vec{k})$ associated with the NDS:

$$\sum_{\ell'} H_{\ell\ell'}(\vec{k}) a_{\ell'}^j(\vec{k}) = E_j(\vec{k}) a_{\ell}^j(\vec{k}), \quad (\text{IIIB8})$$

where

$$H_{\ell\ell'}(\vec{k}) = \left(\frac{\hbar^2 k^2}{2m_0} + \epsilon_{\ell} \right) \delta_{\ell\ell'} + \langle u_{\ell} | \vec{v} | u_{\ell'} \rangle \cdot \hbar \vec{k} + \sum_v \frac{\hbar \vec{k} \cdot \langle u_{\ell} | \vec{v} | u_v \rangle \langle u_v | \vec{v} | u_{\ell'} \rangle \cdot \hbar \vec{k}}{-\epsilon_v}. \quad (\text{IIIB9})$$

The $N \times N$ matrix $H_{\ell\ell'}(\vec{k})$ is the effective mass Hamiltonian, and its j^{th} solution at $\vec{k}$ is the N dimensional eigenvector

$$a^j(\vec{k}) \equiv \begin{pmatrix} a_1^j(\vec{k}) \\ a_2^j(\vec{k}) \\ \vdots \\ a_N^j(\vec{k}) \end{pmatrix}. \quad (\text{IIIE10})$$

The energies ϵ_{ℓ} , the vector quantities $\langle u_{\ell} | \vec{v} | u_{\ell'} \rangle$, and tensor quantities

$$\sum_v \frac{\langle u_{\ell} | \vec{v}_{\alpha} | u_v \rangle \langle u_v | \vec{v}_{\beta} | u_{\ell'} \rangle}{-\epsilon_v}$$

which appear in the effective mass Hamiltonian are treated as parameters to be experimentally determined. Through the use of the symmetry properties of the lattice one may greatly reduce the number of independent parameters involved.

At the end of this section will come a discussion of the modifications which must be made in the presence of a magnetic field. In order to prepare for this discussion, we will put our equations into an equivalent form by replacing $\vec{k}$ by the operator $\vec{p}$ in the effective mass Hamiltonian $H_{\ell\ell}(\vec{k})$ of Eq. IIIB8, and solving

$$\sum_{\ell} H_{\ell\ell}(\vec{p}) F_{\ell}^j(\vec{r}, \vec{k}) = E_j(\vec{k}) F_{\ell}^j(\vec{r}, \vec{k}), \quad (\text{IIIB11})$$

in which case one would find that, when the magnetic field is zero, the appropriate envelope functions $F_{\ell}^j(\vec{r}, \vec{k})$, are related to the expansion coefficients, $a_{\ell}^j(\vec{k})$, by

$$F_{\ell}^j(\vec{r}, \vec{k}) = e^{i\vec{k} \cdot \vec{r}} a_{\ell}^j(\vec{k}), \quad (\text{IIIB12})$$

and the corresponding functions outside of the NDS will become

$$F_{\nu}^j(\vec{r}, \vec{k}) = \sum_{\ell} \frac{\langle u_{\nu} | \vec{v} | u_{\ell} \rangle \cdot \vec{p} F_{\ell}^j(\vec{r}, \vec{k})}{-E_{\nu}}. \quad (\text{IIIB13})$$

Thus, the one electron wave functions and the band edge functions would be related by

$$\psi_{\vec{k}}^j(\vec{r}) = \sum_{\ell} F_{\ell}^j(\vec{r}, \vec{k}) u_{\ell} + \sum_{\nu} F_{\nu}^j(\vec{r}, \vec{k}) u_{\nu}. \quad (\text{IIIB14})$$

At $\vec{k} = 0$, each of the eigenfunctions $\psi^j(\vec{r})$ will contain only one of the functions u_j . In other words, only one envelope function, $F_{\ell}^j(\vec{r}, \vec{k})$ will be nonzero. As we get further and further from $\vec{k}_0$, the band wave functions become more and more mixed, until the approximations in Eqs. IIIB7 and 13 break down, and the effective mass approximation is no longer useful.

We will now find the matrix element of the velocity operator $\vec{v}$ between the eigenfunctions of the one electron Hamiltonian, $\psi_{\vec{k}}^j(\vec{r})$ and $\psi_{\vec{k}}^{j'}(\vec{r})$.

$$\begin{aligned}
\langle \psi_{\vec{k}}^j(\vec{r}) | \vec{v} | \psi_{\vec{k}}^{j'}(\vec{r}) \rangle &= \langle \phi_{\vec{k}}^j(\vec{r}) | \frac{\hbar \vec{k}}{m_0} + \vec{v} | \phi_{\vec{k}}^{j'}(\vec{r}) \rangle \\
&= \langle \sum_{\ell} a_{\ell}^j(\vec{k}) u_{\ell} + \sum_{\nu} a_{\nu}^j(\vec{k}) u_{\nu} | \frac{\hbar \vec{k}}{m_0} + \vec{v} | \sum_{\ell'} a_{\ell'}^{j'}(\vec{k}) u_{\ell'} + \sum_{\nu'} a_{\nu'}^{j'}(\vec{k}) u_{\nu'} \rangle \\
&= \sum_{\ell \ell'} a_{\ell}^{*j}(\vec{k}) a_{\ell'}^{j'}(\vec{k}) (\langle u_{\ell} | \vec{v} | u_{\ell'} \rangle + \frac{\hbar \vec{k}}{m_0} \delta_{\ell \ell'}) \\
&\quad + \sum_{\ell, \nu} a_{\ell}^{*j}(\vec{k}) a_{\nu}^{j'}(\vec{k}) \langle u_{\ell} | \vec{v} | u_{\nu} \rangle + \sum_{\ell', \nu} a_{\nu}^{*j}(\vec{k}) a_{\ell'}^{j'}(\vec{k}) \langle u_{\nu} | \vec{v} | u_{\ell'} \rangle \\
&\quad + 0 ([a_{\nu}^j(\vec{k})]^2). \tag{IIIB15}
\end{aligned}$$

Neglecting the terms of order $[a_{\nu}^j(\vec{k})]^2$, and using the value for $a_{\nu}^j(\vec{k})$ given by Eq. IIIB7, we find

$$\langle \psi_{\vec{k}}^j(\vec{r}) | \vec{v} | \psi_{\vec{k}}^{j'}(\vec{r}) \rangle = \sum_{\ell \ell'} a_{\ell}^{*j}(\vec{k}) \vec{v}_{\ell \ell'}(\vec{k}) a_{\ell'}^{j'}(\vec{k}), \tag{IIIB16}$$

where

$$\begin{aligned}
\vec{v}_{\ell \ell'}(\vec{k}) &= \frac{\hbar \vec{k}}{m_0} \delta_{\ell \ell'} + \langle u_{\ell} | \vec{v} | u_{\ell'} \rangle + \sum_{\nu} \frac{\langle u_{\ell} | \vec{v} | u_{\nu} \rangle \langle u_{\nu} | \vec{v} | u_{\ell'} \rangle}{-\epsilon_{\nu}} \\
&\quad + \sum_{\nu} \frac{\hbar \vec{k} \cdot \langle u_{\ell} | \vec{v} | u_{\nu} \rangle \langle u_{\nu} | \vec{v} | u_{\ell'} \rangle}{-\epsilon_{\nu}} = \frac{\partial}{\partial (\hbar \vec{k})} H_{\ell \ell'}(\vec{k}). \tag{IIIB17}
\end{aligned}$$

This result allows us to calculate all quantities required to find the conductivity, including the crystal momentum dependence of the diagonal and nondiagonal elements of the velocity operator, once we have constructed a suitable effective mass Hamiltonian for the region of the Brillouin zone under consideration. The $N \times N$ matrix, $\vec{v}_{\ell \ell'}(\vec{k})$ is called the effective mass velocity operator.

If we have used Eq. IIIB11 and found the functions $F_{\ell}^j(\vec{r}, \vec{k})$ instead of the coefficients $a_{\ell}^j(\vec{k})$, one may form the appropriate effective mass velocity operator $\vec{v}_{\ell \ell'}(\vec{P})$ by replacing $\hbar \vec{k}$ by $\vec{P}$ wherever it appears in Eq. IIIB17,

and replacing Eq. IIIB16 by

$$\langle \psi_{\vec{k}}^j(\vec{r}) | \vec{v} | \psi_{\vec{k}}^{j'}(\vec{r}) \rangle = \sum_{\ell \ell'} \langle F_{\ell}^j(\vec{r}, \vec{k}) | \vec{v}_{\ell \ell'}(\vec{p}) | F_{\ell'}^{j'}(\vec{r}, \vec{k}) \rangle. \quad (\text{IIIB18})$$

So far we have assumed that no external fields have been applied. If a vector potential $\vec{A}$ is present, we need merely replace $\vec{p}$ by $\vec{\pi} = \vec{p} - e\vec{A}/c$ in Eqs. IIIB11, 13 and 18. If a magnetic field has been applied, one then finds that $\vec{k}$ is no longer a valid quantum number, Eq. IIIB12 is no longer true, and the solutions of IIIB11 are much harder to find than before. Eqs. IIIB13, 14 and 18 still apply, however. The solutions to Eq. IIIB11 in the presence of a magnetic field can be written as $F_{\ell}^j(\vec{r}, n, k_H, y)$ where n denotes the Landau level index, j is the band index, y is the spacial quantum number, and k_H is the crystal momentum parallel to the magnetic field.

Our discussion of the basic theory is now finished. In the remaining sections, the theory of sections A and B will be applied as follows:

- 1) Two effective mass Hamiltonians, one suitable for the holes, and the other suitable for the electrons in bismuth will be derived,
- 2) The solutions to these effective mass Hamiltonians will be found,
- 3) from the effective mass Hamiltonians the corresponding effective mass velocity operators will be derived using Eq. IIIB17,
- 4) using Eq. IIIB18, the matrix elements of the ordinary velocity operator, $\vec{v}$, will be evaluated, and
- 5) the conductivity tensor will be calculated using Eq. IIIA25.

SECTION IIIC

HOLE CONDUCTIVITY

In this section we will use the theory which has been explained in the preceeding two sections to calculate the conductivity tensor for the holes, a problem which has been solved before by other much simpler techniques. (65) Although the calculation presented here is somewhat complicated and unusual, the results we will obtain, although in agreement with the standard expressions, are algebraically much simpler, and display the field dependence of the conductivity in an unusually transparent form. The main reason, however, that we solve the problem in this way is to provide a simple example of the application of the theory of Sections A and B, and to introduce the notation we will use in Section D, where we will require all of the complicated machinery presented here to treat the tightly coupled valence and electronic conduction bands. In our notation, the expression for the conductivity due to the holes is found to be

$$\sigma_{\gamma\beta} = \overset{\leftrightarrow}{C}[1](\sigma_{+-} + \sigma_{-+}) + \overset{\leftrightarrow}{C}[2](\sigma_{+-} - \sigma_{-+}) + \overset{\leftrightarrow}{C}[3]\sigma_{33},$$

where

$$\sigma_{33} = \frac{Ne^2\tau}{(1-i\omega\tau)m_0},$$

$$\sigma_{+-} = \frac{Ne^2\tau}{[1-i\tau(\omega-\omega_c)]m_0},$$

and $\sigma_{-+} = \frac{Ne^2\tau}{[1-i\tau(\omega+\omega_c)]m_0}.$

The three tensors, $\overset{\leftrightarrow}{C}[\ell]$, are determined solely by the effective mass tensor for the carriers and the direction of the magnetic field; m_0 is the free electron mass, and all the other symbols have their usual meanings. The $\overset{\leftrightarrow}{C}[\ell]$ tensors can be defined most simply by the relations:

$$C[1]_{\gamma\beta} = \frac{1}{2}(W_Y[1] W_\beta[1] + W_Y[2] W_\beta[2]),$$

$$C[2]_{\gamma\beta} = \frac{1}{2}(W_Y[2] W_\beta[1] - W_Y[1] W_\beta[2]),$$

and $C[3]_{\gamma\beta} = W_Y[3] W_\beta[3],$

where the nine quantities, $W_Y(j)$ are any set of nine real numbers⁽¹⁰⁾ which satisfy two simple conditions.* The first is that

$$\sum_j W_Y(j) W_\beta(j) = \alpha_{\gamma\beta}^H,$$

where $\alpha_{\gamma\beta}^H$ is the reciprocal effective mass tensor for the holes. The second is that if we define the vectors

$$\vec{W}(j) = \sum_Y \vec{a}_Y W_Y(j),$$

where $\vec{a}_Y$ is a member of a set of three orthonormal unit vectors then

$$\vec{W}(1) \times \vec{W}(3) \cdot \vec{H} = 0,$$

$$\vec{W}(2) \times \vec{W}(3) \cdot \vec{H} = 0,$$

and $\vec{W}(1) \times \vec{W}(2) \cdot \vec{H} < 0.$

In the remainder of this section, we will derive and discuss the expressions above. Our first step is to set up a suitable effective mass Hamiltonian, of a form consistent with experimental observations⁽⁴⁰⁾ and any ab initio band calculations which may be available.⁽¹⁵⁾ This information indicates that the holes lie about the T point in the Brillouin zone,⁽³⁴⁾ and are associated with a simple, nondegenerate band with a parabolic dispersion relation.⁽³⁷⁾ Since we did not find any effects which could be associated with interband transitions involving the hole band, we have assumed that the hole band does not interact strongly with any other band. Therefore, the NDS will contain only the pair of Kravtsov's degenerate band edge functions at T: U_1 and U_2 . The effective mass secular equation for the zero field system can then

* A simple algorithm for choosing the vectors $\vec{W}(j)$ such that these conditions are satisfied is given in Appendix C.

be written, using equation IIIB8,

$$0 = \begin{pmatrix} H_{11}(\vec{k}) - E(\vec{k}) & H_{12}(\vec{k}) \\ H_{21}(\vec{k}) & H_{22}(\vec{k}) - E(\vec{k}) \end{pmatrix} \begin{pmatrix} a_1(\vec{k}) \\ a_2(\vec{k}) \end{pmatrix}. \quad (\text{IIIC1})$$

We will now calculate the effective mass Hamiltonian matrix elements, $H_{ij}(\vec{k})$, in their most general form, subject to the restrictions imposed by symmetry. First we will consider the time reversal conjugation symmetry operator Q , where, ⁽¹⁰⁾

$$Q = i\sigma_2 CI, \quad (\text{IIIC2})$$

where σ_2 is the standard Pauli spin matrix, C is the conjugation operator, and I is the inversion operator. The states U_1 and U_2 are related by the equations

$$U_2 = QU_1 \quad (\text{IIIC3a})$$

$$\text{and } U_1 = -QU_2. \quad (\text{IIIC3b})$$

Similar relations also hold for U_{v1} and U_{v2} , a Kramer's doublet of states where once again, the Greek letters indicate band edge wave functions at T not in the NDS.

It can be easily shown that the velocity operator commutes with Q , and that for any two wave functions ψ and ψ' ,

$$\langle \psi | \vec{v} Q \psi' \rangle = -\langle Q \psi | \vec{v} \psi' \rangle^* = -\langle \psi' | \vec{v} Q \psi \rangle. \quad (\text{IIIC4})$$

One may now calculate the diagonal effective mass Hamiltonian matrix elements using Equation IIIC4 to relate the various velocity matrix elements involved in Eq. IIIB9 of the previous section. One finds ⁽⁶²⁾

$$H_{jj} = -\hbar^2 \vec{k} \cdot \frac{\vec{\alpha}}{2m_0} \cdot \vec{k} + S_j \vec{M}[\vec{k} \times \vec{k}] \frac{c\hbar}{ie}, \quad (\text{IIIC5})$$

where S_j is twice the spin corresponding to state U_j ; $S_1 = +1$, and $S_2 = -1$. There is no term linear in $\vec{k}$ in Eq. IIIC5 because of the inversion symmetry

at the T point. (67)

The expression for $\overleftrightarrow{\alpha}$, the hole reciprocal effective mass tensor is (62)

$$\alpha_{\beta\gamma} = \delta_{\beta\gamma} + 2m_0 \sum_{v,s} [\langle U_1 | v_\gamma | U_{vs} \rangle \langle U_{vs} | v_\beta | U_1 \rangle / \epsilon_v + \langle U_1 | v_\beta | U_{vs} \rangle \langle U_{vs} | v_\gamma | U_1 \rangle / \epsilon_v], \quad (\text{IIIC6})$$

where the first term is a Kroniker delta arising from the kinetic energy of a free particle, and the second is the contribution to the hole effective mass from bands outside the NDS.

The expression for $\vec{M}$ is (25)

$$\vec{M} = \frac{-ie\hbar}{c} \sum_{v,s} \frac{\langle U_1 | \vec{v} | U_{vs} \rangle \times \langle U_{vs} | \vec{v} | U_1 \rangle}{\epsilon_v}. \quad (\text{IIIC7})$$

If there is no magnetic field, $\vec{k}$ is not an operator and $\hbar \vec{k} \times \hbar \vec{k} = 0$.

If we do have a magnetic field, we replace $\hbar \vec{k}$ by $\vec{\pi} = \vec{p} - \frac{e\vec{A}}{c}$, so that

$\vec{\pi} \times \vec{\pi} = ie\hbar\vec{H}/c$. (62) We may now write the diagonal matrix elements

$$H_{jj}(\vec{\pi}) = -\vec{\pi} \cdot \frac{\overleftrightarrow{\alpha}}{2m_0} \cdot \vec{\pi} + S_j \vec{M} \cdot \vec{H}. \quad (\text{IIIC8})$$

Due to the trigonal symmetry (67) at the T point: a) $\vec{M}$ must be parallel to

the trigonal axis; b) $\alpha_{xy} = \alpha_{yx} = \alpha_{xz} = \alpha_{yz} = \alpha_{zy} = 0$; and c) $\alpha_{yy} = \alpha_{xx}$.

One can carry out the same steps for the off-diagonal elements and find that in the presence of a field, the two states of the Kramers doublet are coupled, and

$$H_{12}(\vec{\pi}) = H_{21}^*(\vec{\pi}) = \mathcal{L} \cdot \vec{H}, \quad (\text{IIIC9})$$

where

$$\mathcal{L} = \frac{-ie\hbar}{c} \sum_v \frac{\langle U_1 | \vec{v} | U_{v1} \rangle \times \langle U_{v1} | \vec{v} | U_2 \rangle}{\epsilon_v}. \quad (\text{IIIC10})$$

The effective mass Hamiltonian may now be written

$$\begin{aligned}
H &= \begin{pmatrix} -\vec{\pi} \cdot \frac{\vec{\alpha}}{2m_0} \cdot \vec{\pi} + \vec{M} \cdot \vec{H} & \vec{\mathcal{L}} \cdot \vec{H} \\ \vec{\mathcal{L}}^* \cdot \vec{H} & -\vec{\pi} \cdot \frac{\vec{\alpha}}{2m_0} \cdot \vec{\pi} + \vec{M} \cdot \vec{H} \end{pmatrix} \\
&= -\vec{\pi} \cdot \frac{\vec{\alpha}}{2m_0} \cdot \vec{\pi} \sigma_0 + \sum_j \sigma_j L_j,
\end{aligned} \tag{IIIC11}$$

where σ_0 is the unit 2x2 matrix, σ_1 , σ_2 and σ_3 are the Pauli spin matrices, and

$$L_1 \equiv \vec{H} \cdot \text{Re}\{\vec{\mathcal{L}}\}, \tag{IIIC12a}$$

$$L_2 \equiv -\vec{H} \cdot \text{Im}\{\vec{\mathcal{L}}\}, \tag{IIIC12b}$$

$$L_3 \equiv \vec{H} \cdot \vec{M}. \tag{IIIC12c}$$

Using Equation IIIB17, we may now write the corresponding effective mass velocity operator

$$\mathbf{v} = \frac{-1}{m_0} \begin{pmatrix} \vec{\alpha} \cdot \vec{\pi} & 0 \\ 0 & \vec{\alpha} \cdot \vec{\pi} \end{pmatrix} = -\frac{\vec{\alpha} \cdot \vec{\pi} \sigma_0}{m_0}. \tag{IIIC13}$$

In order to calculate the conductivity tensor using Eq. IIIA25, we must find: a) the eigenvalues of the effective mass Hamiltonian IIIC11; and b) the velocity matrix elements between the corresponding eigenstates. There are many ways to do this. The method we will use has been chosen for its similarity to the method we will use for the bands associated with the electrons.

First, let us define three real vectors $\vec{W}(1)$, $\vec{W}(2)$, and $\vec{W}(3)$ by the relation⁽¹⁰⁾

$$\sum_{j=1}^3 W_p(j) W_\gamma(j) \equiv \alpha_{\beta\gamma}, \tag{IIIC14}$$

where $\vec{\alpha}$ is the previously defined reciprocal effective mass tensor. If $H = 0$, the three vectors are otherwise completely arbitrary. If $H \neq 0$, it

is convenient to specify the vectors more completely. We will discuss this point more fully a bit further on. Assuming the three vectors, $\vec{W}(j)$ have been chosen, we may define

$$P_j \equiv \sqrt{\frac{1}{m_0}} \vec{W}(j) \cdot \vec{\pi} . \quad (\text{IIIC15})$$

If we consider the quantities P_j , σ_j and L_j as the components of a vector in a transformed space, we may use vector notation to simplify the form of the Hamiltonian, and write

$$H = - \frac{P^2}{2} \sigma_0 + \vec{L} \cdot \vec{\sigma} . \quad (\text{IIIC16})$$

In this notation, the velocity operator of Equation IIIC13 becomes

$$\vec{V} = - \sum_j \vec{W}(j) \frac{P_j \sigma_0}{\sqrt{m_0}} = \sum_j \vec{W}(j) \chi(j) . \quad (\text{IIIC17})$$

The above expression defines the three 2x2 matrix operators $\chi(j)$, which can be considered to be the components of a velocity operator in the transformed space. We will first work out the conductivity when $H = 0$. In this case, the Hamiltonian is completely diagonal, and one may quite easily find the necessary eigenvalues and matrix elements. There are two degenerate solutions to H , required by time reversal symmetry, with eigenvalues

$$-\frac{K^2}{2} = E_1(\vec{K}) = E_2(\vec{K}) , \quad (\text{IIIC18})$$

where

$$K_j \equiv \vec{W}(j) \cdot \vec{k} \hbar / \sqrt{m_0} \quad (\text{IIIC19})$$

is a component of a vector in the transformed space. The corresponding eigenvectors of the effective mass Hamiltonian may be written

$$a^1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad (\text{IIIC20})$$

and $a^2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad (\text{IIIC21})$

To calculate the conductivity it is not necessary to explicitly calculate the one electron wave functions, ψ_1 and ψ_2 , though it is possible to do so using the techniques of the previous chapter. Using Eq. IIIB16, we may write

$$\langle \psi_1 | \vec{v} | \psi_2 \rangle = \langle \psi_2 | \vec{v} | \psi_1 \rangle = 0, \quad (\text{IIIC22})$$

and

$$\langle \psi_2 | \vec{v} | \psi_2 \rangle = \langle \psi_1 | \vec{v} | \psi_1 \rangle = \sum_j - \frac{\vec{W}(j) K_j}{m_0}. \quad (\text{IIIC23})$$

Since the velocity matrix element is completely diagonal in all quantum numbers, we must replace $\frac{f_i - f_j}{E_i - E_j}$ in Eq. IIIA25 by $\frac{df(E)}{dE}$ as discussed in connection with Eq. IIIA13. The contributions to the conductivity from the two spin states are identical, so substituting in Eq. IIIA25, we get

$$\sigma_{\gamma\beta} = \frac{-2e^2\tau}{m_0(1-i\omega\tau)} \sum_{\vec{K}} \frac{df(E)}{dE} \sum_{j\ell} W_\gamma(j) W_\beta(\ell) K_j K_\ell. \quad (\text{IIIC24})$$

We get no contribution for $j \neq \ell$ because $\frac{df(E)}{dE}$ is a function of K^2 only.

In order to concentrate on carrying out the sum over $\vec{K}$, we will write

$$\sigma_{\gamma\beta} = \sum_j W_\gamma(j) W_\beta(j) \sigma_0(j), \quad (\text{IIIC25})$$

where

$$\sigma_0(j) = \frac{-2e^2\tau}{m_0(1-i\omega\tau)} \sum_{\vec{K}} \frac{df(E)}{dE} K_j^2. \quad (\text{IIIC26})$$

It is clear that $\sigma_0(1) = \sigma_0(2) = \sigma_0(3)$. To evaluate $\sigma_0(3)$, we convert the sum to an integral

$$\begin{aligned} \sigma_0(3) &= \frac{-2e^2 C_K \tau}{m_0(1-i\omega\tau)} \int d\vec{K} \frac{df(E)}{dE} K_3^2 \\ &= \frac{-8\pi e^2 C_K \tau}{m_0(1-i\omega\tau)} \int_0^\infty K^4 \frac{df(E)}{dE} dK. \end{aligned} \quad (\text{IIIC27})$$

Here C_K is the factor which takes into account the density of states involved in conversion from the sum to the integral. It is defined by the requirement

$$N = 2C_K \int d\vec{K} (1-f(E)) = 8\pi C_K \int_0^\infty K^2 dK (1-f(E)), \quad (\text{IIIC28})$$

where N is the hole concentration.

It can be shown that

$$3 \int_0^\infty K^2 dK (1-f(E)) = - \int_0^\infty K^4 \frac{df(E)}{dE}, \quad (\text{IIIC29})$$

so that we may now combine equations IIIC27 and C28 to find

$$\sigma_0(3) = \frac{Ne^2 \tau}{(1-i\omega\tau)m_0} \quad (\text{IIIC30})$$

Finally, we may write the conductivity tensor

$$\sigma_{\gamma\beta} = \sum_j W_\gamma(j) W_\beta(j) \frac{Ne^2 \tau}{m_0(1-i\omega\tau)} = \frac{\alpha_{\gamma\beta} Ne^2 \tau}{(1-i\omega\tau)m_0} \quad (\text{IIIC31})$$

This is the same equation which can, of course, be derived in a much simpler way. (65)

To work out the conductivity when $H \neq 0$ we must first solve the effective mass Hamiltonian of Eq. IIIC11. We will first find the eigenvalues of P^2 , the only non C number in the Hamiltonian. To do this, we must first find the commutator

$$\begin{aligned} [P_i, P_j] &= \frac{1}{2m_0} \sum_{\gamma\beta} [W_\gamma(i)\pi_\gamma, W_\beta(j)\pi_\beta] + [W_\beta(i)\pi_\beta, W_\gamma(j)\pi_\gamma] \\ &= \frac{1}{2m_0} \sum_{\gamma\beta} [W_\gamma(i)W_\beta(j) - W_\beta(i)W_\gamma(j)] [\pi_\gamma\pi_\beta - \pi_\beta\pi_\gamma] \\ &= [\vec{W}(i) \times \vec{W}(j)] \cdot \frac{[\vec{\pi} \times \vec{\pi}]}{m_0} = i[\vec{W}(i) \times \vec{W}(j)] \cdot \vec{H} \frac{e\hbar}{m_0 c} \end{aligned} \quad (\text{IIIC32})$$

or, treating the P_j and b_j as vectors in the transformed space, Eq. IIIC32 can be written as (10)

$$\vec{P} \times \vec{P} = i\vec{b}, \quad (\text{IIIC33})$$

where

$$b_{\ell} = \sum_{ij} [\vec{W}(i) \times \vec{W}(j)] \cdot \vec{H} \frac{e\hbar}{m_0 c} \bar{e}_{ij\ell}, \quad (\text{IIIC34})$$

where $\bar{\epsilon}_{ijl}$ is the positive part of the completely antisymmetric tensor,

ϵ_{ijl} .

In order to simplify the calculation it is convenient to pick the three vectors, $\vec{W}(j)$, such that $b_1 = b_2 = 0$, and b_3 is positive. It will be seen that in this case, $b_3 = \hbar\omega_c$. Note that here, as everywhere in the derivation, e is the signed charge of the electron, so that we require $\vec{W}(1) \times \vec{W}(2) \cdot \vec{H}$ to be negative.

We now may proceed in the standard way,⁽⁶⁸⁾ and find that the eigenvalues, λ , of P^2 are

$$\lambda = (2n+1) b_3 + K_3^2, \quad (\text{IIIC35})$$

where n is the Landau level index. The corresponding harmonic oscillator eigenfunctions may be written $\phi(n, K_3)$.

Because of the orthogonality of the harmonic oscillator functions, the effective mass Hamiltonian (Eq. IIIC11) does not connect states of different n and K_3 , so we may write $F^j(n, K_3)$, the j^{th} solution to the effective mass secular equation, in the form

$$F^j(n, K_3) \begin{pmatrix} F_1^j(n, K_3) \\ F_2^j(n, K_3) \end{pmatrix} = \begin{pmatrix} a_1^j \\ a_2^j \end{pmatrix} \phi(n, K_3) = a^j \phi(n, K_3), \quad (\text{IIIC36})$$

where $F_1^j(n, K_3)$ are the envelope functions defined by Eq. IIIB12, and a^j is the spin eigenvector. Upon substitution of this form into the secular equation, we find we must solve

$$0 = \begin{pmatrix} -E - \lambda/2 + \vec{M} \cdot \vec{H} & \vec{L} \cdot \vec{H} \\ \vec{L}^* \cdot \vec{H} & -E - \lambda/2 - \vec{M} \cdot \vec{H} \end{pmatrix} \begin{pmatrix} a_1^j \\ a_2^j \end{pmatrix} \\ = \{ -(E + \lambda/2)\sigma_0 + \vec{L} \cdot \vec{\sigma} \} a^j. \quad (\text{IIIC37})$$

This may be easily done to yield

$$E_j^{\pm} = -\lambda/2 \pm \sqrt{\sum L_j^2} = -\lambda/2 \pm \sqrt{\vec{H} \cdot \vec{G} \cdot \vec{H}} \quad , \quad (\text{IIIC38})$$

where

$$G_{\gamma\beta} = M_{\gamma} M_{\beta} + \mathcal{L}_{\gamma} \mathcal{L}_{\beta}^* \quad . \quad (\text{IIIC39})$$

The effective g factor, g^* , then will be given ⁽²⁹⁾ by the expression

$$g^* = \frac{4\mu_B \vec{G}}{\hbar e H} \sqrt{\vec{H} \cdot \vec{G} \cdot \vec{H}} \quad . \quad (\text{IIIC40})$$

The eigenvectors of IIIC37 are

$$\begin{pmatrix} a_1^j \\ a_2^j \end{pmatrix} = \frac{1}{\sqrt{(E_j + \lambda/2 - \vec{M} \cdot \vec{H})^2 + |\mathcal{L} \cdot \vec{H}|^2}} \begin{pmatrix} E_j + \lambda/2 - \vec{M} \cdot \vec{H} \\ \mathcal{L} \cdot \vec{H} \end{pmatrix} \quad . \quad (\text{IIIC41})$$

The corresponding one electron wave functions, $\psi_1(n, K_3)$ and $\psi_2(n, K_3)$ can be found using IIIB14. Due to the trigonal symmetry at point T: a) $G_{xx} = G_{yy}$ and b) $G_{xy} = G_{xz} = G_{yz} = G_{zx} = G_{zy} = G_{yz} = 0$. Note that since different combinations of interband matrix elements are involved in $\vec{G}$ and $\vec{\alpha}$ (see Eqs. IIIC6, 7 and 10), one tensor is not determined by the other.

In order to evaluate the velocity matrix elements appearing in Eq. IIIA25, it is most convenient to define ⁽¹⁰⁾

$$P_{\pm} = \frac{P_1 \pm i P_2}{\sqrt{2}} \quad , \quad (\text{IIIC42})$$

and also define $\chi(\pm)$ and $\vec{W}(\pm)$ by similar relations. One may now rewrite the effective mass velocity operator.

$$\vec{V} = (\vec{W}(+) \chi(-) + \vec{W}(-) \chi(+) + \vec{W}(3) \chi(3)) \quad . \quad (\text{IIIC43})$$

To evaluate this expression, we can find, by the standard harmonic oscillator derivation, ⁽⁶⁸⁾ that

$$\sqrt{b_3 n} \phi(n-1, K_3) = P_+ \phi(n, K_3) \quad , \quad (\text{IIIC44})$$

$$\sqrt{b_3 (n+1)} \phi(n+1, K_3) = P_- \phi(n, K_3) \quad , \quad (\text{IIIC45})$$

and

$$K_3 \phi(n, K_3) = P_3 \phi(n, K_3) . \quad (\text{IIIC46})$$

Since the three 2x2 matrix operators, $\chi(\ell)$, are diagonal in spin, we find

$$\langle F^j(n, K_3) | \chi(+)| F^j(n', K'_3) \rangle = -\sigma_{jj} \sigma_{K_3 K'_3} \sigma_{n, n'-1} \sqrt{\frac{b_3(n+1)}{m_0}} , \quad (\text{IIIC47})$$

$$\langle F^j(n, K_3) | \chi(-)| F^j(n', K'_3) \rangle = -\sigma_{jj} \sigma_{K_3 K'_3} \sigma_{n, n'+1} \sqrt{\frac{b_3 n}{m_0}} , \quad (\text{IIIC48})$$

and

$$\langle F^j(n, K_3) | \chi(3)| F^j(n', K'_3) \rangle = -\sigma_{jj} \sigma_{K_3 K'_3} \sigma_{n, n'} \frac{K_3}{\sqrt{m_0}} . \quad (\text{IIIC49})$$

Before we substitute these expressions into Eq. IIIA25, let us define some convenient notation. Instead of $F^j(n, K_3)$ we will write $F(z)$ where z stands for the state defined by quantum numbers j , n , and K_3 . Other subscripted quantities can be handled similarly. We may also write the expression $\langle \psi(z) | v_Y | \psi(z') \rangle \langle \psi(z') | v_\beta | \psi(z) \rangle$ which appears in Eq. IIIA25 in a more convenient form,

$$\begin{aligned} & \langle \psi(z) | v_Y | \psi(z') \rangle \langle \psi(z') | v_\beta | \psi(z) \rangle \\ &= \langle F(z) | W_Y(+) \chi(-) + W_Y(-) \chi(+) + W_Y(3) \chi(3) | F(z') \rangle \\ & \times \langle F(z') | W_\beta(+) \chi(-) + W_\beta(-) \chi(+) + W_\beta(3) \chi(3) | F(z) \rangle \\ &= W_Y(+) W_\beta(-) \langle F(z) | \chi(-) | F(z') \rangle \langle F(z') | \chi(+) | F(z) \rangle \\ &+ W_Y(-) W_\beta(+) \langle F(z) | \chi(+) | F(z') \rangle \langle F(z') | \chi(-) | F(z) \rangle \\ &+ W_Y(3) W_\beta(3) | \langle F(z) | \chi(3) | F(z') \rangle |^2 . \end{aligned} \quad (\text{IIIC50})$$

We may now proceed in a similar manner as for $H = 0$, and use Equation IIIA25 to find an expression for $\sigma_{Y\beta}$

$$\sigma_{Y\beta} = W_Y(+) \sigma_{-} W_\beta(-) + W_Y(-) \sigma_{-} W_\beta(+) + W_Y(3) \sigma_{33} W_\beta(3)$$

$$= \frac{1}{2}(W_Y[1]W_B[1] + W_Y[2]W_B[2])(\sigma_{+-} + \sigma_{-+}) \\ + \frac{1}{2}(W_Y[2]W_B[1] - W_Y[1]W_B[2])(\sigma_{+-} - \sigma_{-+}) + W_Y(3)W_B(3)\sigma_{33} , \quad (\text{IIIC51})$$

where

$$\sigma_{+-} = -e^2 \sum_{zz'} \frac{(f[z]-f[z'])\langle F(z)|\chi(-)|F(z')\rangle\langle F(z')|\chi(+)|F(z)\rangle}{(E[z]-E[z'])\left(-i\omega + \frac{1}{\tau} + \frac{i}{K}[E(z')-E(z)]\right)} , \quad (\text{IIIC52})$$

and σ_{-+} is similarly defined, with $\chi(-)$ and $\chi(+)$ interchanged. Since $\chi(3)$ is completely diagonal, we must replace $\frac{f(s)-f(s')}{E(s)-E(s')}$, by $\frac{df(E)}{dE}$ to find

$$\sigma_{33} = -e^2 \sum_z \frac{d[f(E)/dE]|\langle F(z)|\chi(3)|F(z)\rangle|^2}{\left(\frac{1}{\tau} - i\omega\right)} . \quad (\text{IIIC53})$$

We will first work out σ_{33} . Substituting the proper expressions for the matrix elements

$$\sigma_{33} = -e^2 \sum_{K_3, n, j} \frac{df(E)}{dE} \frac{K_3^2}{\left(\frac{1}{\tau} - i\omega\right)m_0} . \quad (\text{IIIC54})$$

We may now replace the sum by an integral, and find

$$\sigma_{33} = -\frac{e^2 C_K \tau}{(1-i\omega\tau)m_0} \sum_{n, j} \int_0^\infty dK_3 K_3^2 \frac{df(E)}{dE} , \quad (\text{IIIC55})$$

where, once again, C_K is the normalization constant, and we require

$$N = C_K \sum_{n, j} \int_0^\infty (1-f(E))dK_3 , \quad (\text{IIIC56})$$

where N is the density of holes. Using a technique similar to the one used for the $H = 0$ case, we may show

$$\int_0^\infty dK_3 K_3^2 \frac{df(E)}{dE} = - \int_0^\infty (1-f(E))dK_3 , \quad (\text{IIIC57})$$

so that

$$\sigma_{33} = \frac{Ne^2 \tau}{(1-i\omega\tau)m_0} . \quad (\text{IIIC58})$$

We will now work out σ_{+-} . In this case, the matrix elements are nonzero only when $n+1 = n'$, so that

$$\begin{aligned}\sigma_{+-} &= -e^2 \sum_{j, K_3} \frac{[f(E_j(n, K_3)) - f(E_j(n+1, K_3))] b(n+1)}{m_o [E_j(n, K_3) - E_j(n+1, K_3)] \left[\frac{1}{\tau} - i\omega + \frac{i}{\hbar} (E_j(n, K_3) - E_j(n+1, K_3)) \right]} \\ &= -e^2 \sum_{j, K_3} \frac{[f(E_j(n, K_3)) - f(E_j(n+1, K_3))] b(n+1)}{b \left[\frac{1}{\tau} - i\omega + ib/\hbar \right] m_o} \quad (\text{IIIC59})\end{aligned}$$

Since

$$\begin{aligned}\sum_{j, K_3, n=0}^{n=\infty} (f(E_j(n, K_3)) - f(E_j(n+1, K_3))) (n+1) \\ = \sum_{j, K_3, n=0}^{n=\infty} \{f(E_j(n, K_3)) - 1\} = -N, \quad (\text{IIIC60})\end{aligned}$$

where N is the density of holes,

$$\sigma_{+-} = \frac{e^2 N \tau}{m_o (1 - i\tau(b_3/\hbar - \omega))} \quad (\text{IIIC61})$$

In a similar manner it may be shown that

$$\sigma_{-+} = \frac{e^2 N \tau}{m_o (1 - i\tau(b_3/\hbar + \omega))} \quad (\text{IIIC62})$$

By comparison with the standard expression, ^(33,37) we thus see that b_3 must equal $|\hbar\omega_c|$ so that

$$b_3 = \frac{\hbar |e| (\vec{H} \cdot \vec{m}^* \cdot \vec{H})^{1/2}}{m_o c |\vec{m}^*|^{1/2}} \equiv \beta^* H, \quad (\text{IIIC63})$$

which defines β^* , where $\vec{m}^* = (\alpha)^{-1}$ is the effective mass tensor. This equation may also be proven from the definition of b_3 after a considerable amount of labor. A similar comparison between the role of K_3^2 in Eqs. IIIC35 and IIIC38, and the role of K_H^2 in the standard expressions shows

$$K_3^2 = k_H^2 / m_H m_o, \quad (\text{IIIC64})$$

where

$$m_H = (\vec{H} \cdot \vec{m}^* \cdot \vec{H}) / H^2, \quad (\text{IIIC65})$$

and k_H is the crystalline momentum parallel to the magnetic field. Eqs.

IIIC64 and IIIC65 are proven in Section IIIE.

We now have completely evaluated the contribution to the conductivity tensor from the holes, for arbitrary temperature with arbitrary spin-orbit coupling. In the next section we will apply the techniques illustrated here to find the contribution to the conductivity tensor arising from the two band model for the electrons. In this section, our walnut will be more in keeping with the size of our hammer.

SECTION IIID

THE CONDUCTIVITY DUE TO THE ELECTRONS

In this section, we will derive an expression for the contribution to the conductivity from the tightly coupled valence and conduction bands associated with the electrons. We will consider only the principal ellipsoid for simplicity, but the formulas derived here may also be used for the non-principal ellipsoids by performing a rotation of $\pm 120^\circ$ about the trigonal axis. It should be pointed out that the conductivity associated with each of the three ellipsoids will be different for a general direction of magnetic field.

Our first step in the calculation will be to derive an appropriate effective mass Hamiltonian of the most general form, which we will call the Baraff Hamiltonian.⁽³⁹⁾ Discarding certain small terms we will find a simpler effective mass Hamiltonian which we will call the Wolff Hamiltonian.⁽¹⁰⁾ This is the Hamiltonian appropriate to the two band model of Lax. We will use this Wolff Hamiltonian to calculate the conductivity using the method of Section IIIC. The more complete Baraff Hamiltonian will be discussed in Section IIIE.

We will first derive the Baraff Hamiltonian. The NDS (nearly degenerate subset of bands) must contain at least two bands to yield the nonparabolic behavior observed in the magnetoreflexion experiments.⁽³⁾ These bands must be nondegenerate because there are no degeneracies at the L points in the Brillouin zone.⁽⁶⁷⁾ The reasons for placing the band extrema at the L points have been considered in Chapter I. Since the only oscillations observed in the magnetoreflexivity are due to transitions between the valence and conduction bands, we will assume that these are the only two tightly coupled

bands, and form the NDS. When the electron spin is included we then have four band edge wave functions in the NDS: U_{cs} and U_{vs} , where c and v label the conduction and valence bands, and s labels the two members of the Kramers doublet.

The Baraff Hamiltonian is thus a 4x4 matrix, where, using the same techniques as were used for the holes we find

$$H_{11} = \epsilon + \frac{\vec{\pi} \cdot \vec{\beta}^c \cdot \vec{\pi}}{2m_0} + \vec{H} \cdot \vec{M}^c, \quad (\text{IIID1a})$$

and

$$H_{22} = \epsilon + \frac{\vec{\pi} \cdot \vec{\beta}^c \cdot \vec{\pi}}{2m_0} - \vec{H} \cdot \vec{M}^c, \quad (\text{IIID1b})$$

where

$$\epsilon = E_g/2, \quad (\text{IIID2})$$

and E_g is the energy gap between the conduction and valence bands.

Similarly, we may write

$$H_{12} = \vec{Y}^c \cdot \vec{H}, \quad (\text{IIID3a})$$

$$H_{21} = \vec{Y}^{c*} \cdot \vec{H}, \quad (\text{IIID3b})$$

$$H_{33} = -\epsilon + \frac{\vec{\pi} \cdot \vec{\beta}^v \cdot \vec{\pi}}{2m_0} + \vec{M}^v \cdot \vec{H}, \quad (\text{IIID3c})$$

$$H_{44} = -\epsilon + \frac{\vec{\pi} \cdot \vec{\beta}^v \cdot \vec{\pi}}{2m_0} - \vec{M}^v \cdot \vec{H}, \quad (\text{IIID3d})$$

$$H_{34} = \vec{Y}^v \cdot \vec{H}, \quad (\text{IIID3e})$$

and

$$H_{43} = \vec{Y}^{v*} \cdot \vec{H}. \quad (\text{IIID3f})$$

Using the time reversal conjugation operator, Q, discussed in Section

IIIC, we may show

$$\vec{t} = \langle U_{c1} | \vec{v} | U_{v1} \rangle = \langle U_{c2} | \vec{v} | U_{v2} \rangle^*, \quad (\text{IIID4a})$$

and

$$\vec{u} = \langle U_{c1} | \vec{v} | U_{v2} \rangle = -\langle U_{c2} | \vec{v} | U_{v1} \rangle^* , \quad (\text{IIID4b})$$

and then write

$$H_{13} = \vec{t} \cdot \vec{\pi} , \quad (\text{IIID5a})$$

$$H_{14} = \vec{u} \cdot \vec{\pi} , \quad (\text{IIID5b})$$

$$H_{23} = -\vec{u}^* \cdot \vec{\pi} , \quad (\text{IIID5c})$$

$$H_{24} = \vec{t}^* \cdot \vec{\pi} , \quad (\text{IIID5d})$$

$$H_{31} = \vec{t}^* \cdot \vec{\pi} , \quad (\text{IIID5e})$$

$$H_{41} = \vec{u}^* \cdot \vec{\pi} , \quad (\text{IIID5f})$$

$$H_{32} = -\vec{u} \cdot \vec{\pi} , \quad (\text{IIID5g})$$

and

$$H_{42} = \vec{t} \cdot \vec{\pi} . \quad (\text{IIID5h})$$

There are no terms in Eq. IIID5 quadratic in $\vec{\pi}$ because the valence and conduction bands must have opposite parity.

Using: a) the definitions

$$\mathcal{L}_1^c = R_e \{ \vec{Y}^c \cdot \vec{H} \} , \quad (\text{IIID6a})$$

$$\mathcal{L}_2^c = -I_m \{ \vec{Y}^c \cdot \vec{H} \} , \quad (\text{IIID6b})$$

and

$$\mathcal{L}_3^c = \vec{M}^c \cdot \vec{H} , \quad (\text{IIID6c})$$

with similar definitions for $\mathcal{L}_j^v$; b) the fact, demonstrated by Wolff,⁽¹⁰⁾ that we may always choose a basis such that

$$R_e \{ \vec{t} \} = 0 ; \quad (\text{IIID7})$$

and c) the definitions

$$\vec{X}(1) = \mathbf{I}_m \{\vec{u}\} \sqrt{m_0/\epsilon} , \quad (\text{IIID8a})$$

$$\vec{X}(2) = \mathbf{R}_e \{\vec{u}\} \sqrt{m_0/\epsilon} , \quad (\text{IIID8b})$$

and

$$\vec{X}(3) = \mathbf{I}_m \{\vec{t}\} \sqrt{m_0/\epsilon} ; \quad (\text{IIID8c})$$

we may write the Baraff Hamiltonian

$$H = \sum_{j=1}^3 \begin{pmatrix} \epsilon + \frac{\vec{\pi} \cdot \vec{\beta}^c \cdot \vec{\pi}}{2m_0} + \sigma_j \mathcal{A}_j^c & i\sigma_j \vec{X}(j) \cdot \vec{\pi} \sqrt{\frac{\epsilon}{m_0}} \\ -i\sigma_j \vec{X}(j) \cdot \vec{\pi} \sqrt{\frac{\epsilon}{m_0}} & -\epsilon + \frac{\vec{\pi} \cdot \vec{\beta}^v \cdot \vec{\pi}}{2m_0} + \sigma_j \mathcal{A}_j^v \end{pmatrix} , \quad (\text{IIID9})$$

where σ_j are the Pauli spin matrices.

The tensors $\vec{\beta}^c$ and $\vec{\beta}^v$, and the quantities $\mathcal{A}_j^c$ and $\mathcal{A}_j^v$ essentially describe the interaction between bands inside the NDS and those outside of it. In the two band model of Lax, we assume that all these terms are zero. (35) If we make this assumption we get the Wolff Hamiltonian (10)

$$H_0 = \sum_{j=1}^3 \begin{pmatrix} \epsilon & i\sigma_j \vec{X}(j) \cdot \vec{\pi} \sqrt{\frac{\epsilon}{m_0}} \\ -i\sigma_j \vec{X}(j) \cdot \vec{\pi} \sqrt{\frac{\epsilon}{m_0}} & -\epsilon \end{pmatrix} , \quad (\text{IIID10})$$

which may be exactly diagonalized, even in the presence of a magnetic field, in contrast to the Baraff Hamiltonian, which cannot.

The Lax model is found to predict the resonances in the magneto-reflectivity very well. The giant quantum oscillation experiments of Mase (38) also indicate that the departures from this model, though observable, are small. Therefore we will first work out the conductivity using this approximation, which greatly simplifies the problem.* The

* Except for our introduction of the rotation matrix, $\vec{R}$, we follow the calculation of Wolff (10) in our derivation of the eigenfunctions of H_0 , and the corresponding velocity matrix elements evaluated between these eigenfunctions.

required effective mass velocity operator $\vec{V}_0$, which corresponds to the Wolff Hamiltonian is (10)

$$\vec{V}_0 = \sum_{j=1}^3 \begin{pmatrix} 0 & i\sigma_j \vec{X}(j) \\ -i\sigma_j \vec{X}(j) & 0 \end{pmatrix} \sqrt{\frac{\epsilon}{m_0}} . \quad (\text{IIID11})$$

Let us first find the conductivity when $H = 0$. We must first find the eigenvalues, E_m , and the four component eigenvectors, a^m , by solving the secular equation,

$$0 = \sum_{j=1}^3 \begin{pmatrix} \epsilon - E_m & i\sigma_j \vec{X}(j) \cdot \vec{k} \hbar \sqrt{\frac{\epsilon}{m_0}} \\ -i\sigma_j \vec{X}(j) \cdot \vec{k} \hbar \sqrt{\frac{\epsilon}{m_0}} & -\epsilon - E_m \end{pmatrix} \begin{pmatrix} a^m \end{pmatrix} . \quad (\text{IIID12})$$

We find that there are two eigenvalues, E_+ and E_- , each one doubly degenerate as is required by time reversal symmetry, where

$$E_{\pm} = \pm \hat{\epsilon} , \quad (\text{IIID13})$$

and

$$\hat{\epsilon} = \sqrt{\epsilon^2 + \frac{\hbar^2 \epsilon}{m_0} \sum_j \vec{k} \cdot \vec{X}(j) \vec{X}(j) \cdot \vec{k}} . \quad (\text{IIID14})$$

If $|E_{\pm}|$ is close to ϵ , we find that approximately

$$E_{\pm} = \pm \left(\epsilon + \frac{\hbar^2}{2m_0} \sum_j \vec{k} \cdot \vec{X}(j) \vec{X}(j) \cdot \vec{k} \right) . \quad (\text{IIID15})$$

Therefore, we see that the band is parabolic very close to the extremum, with a reciprocal effective mass tensor $\overleftrightarrow{\alpha}$, given by the equation

$$\alpha_{\beta\gamma} = \sum_j X_{\beta}(j) X_{\gamma}(j) . \quad (\text{IIID16})$$

Therefore, as in Section IIIC, let us write

$$\frac{\vec{X}(j) \cdot \vec{\pi}}{\sqrt{m_0}} \equiv p_j , \quad (\text{IIID17a})$$

and

$$\frac{\vec{X}(j) \hbar k}{\sqrt{m_0}} K_j \quad . \quad (\text{IIID17b})$$

Treating K_j , P_j , or σ_j as the components of vectors in the transformed space, we may write $\hat{\epsilon}$ and H_0 as

$$\hat{\epsilon} = \sqrt{\epsilon^2 + \epsilon K^2} \quad , \quad (\text{IIID18a})$$

and

$$H_0 = \begin{pmatrix} \epsilon & i\sqrt{\epsilon} \vec{P} \cdot \vec{\sigma} \\ -i\sqrt{\epsilon} \vec{P} \cdot \vec{\sigma} & -\epsilon \end{pmatrix} \quad (\text{IIID18b})$$

and the four component eigenvector, $a^j(\vec{K}, S)$ as

$$a^j(\vec{K}, S) = \sqrt{\frac{E_j + \epsilon}{2E_j}} \begin{pmatrix} \ell(S) \\ \frac{-i\vec{K} \cdot \vec{\sigma} \sqrt{\epsilon}}{E_j + \epsilon} \ell(S) \end{pmatrix} \quad , \quad (\text{IIID19})$$

where $j = +$ and $-$ label conduction and valence bands, respectively, and $\ell(1)$ and $\ell(-1)$ are two orthogonal spinors (two component quantities.) It can be shown that $a^j(\vec{K}, 1)$ and $a^j(\vec{K}, -1)$ are related by time reversal symmetry, so that S truly labels the spin. The effective mass velocity operator $\vec{V}_0$ may be written

$$\vec{V}_0 = \sum_j \vec{X}(j) \chi(j) \quad , \quad (\text{IIID20})$$

where

$$\chi(j) = \sqrt{\frac{\epsilon}{m_0}} \begin{pmatrix} 0 & i\sigma_j \\ -i\sigma_j & 0 \end{pmatrix} \quad (\text{IIID21})$$

As before, $\chi(j)$ may be considered to be a component of the velocity vector in the transformed space, and Eq. IIID21 may be written in the alternate form

$$\vec{X}(j) = \sqrt{\frac{\epsilon}{m_0}} \begin{pmatrix} 0 & i\vec{\sigma} \\ -i\vec{\sigma} & 0 \end{pmatrix} \quad (\text{IIID22})$$

To evaluate the velocity operator between the solutions given by Eq. IIID19, we write, since $\vec{\chi}$ is diagonal in $\vec{k}$,

$$\begin{aligned}
& \langle a^j(\vec{k}, S) | \vec{\chi} | a^{j'}(\vec{k}, S') \rangle \\
&= \gamma \left\langle \frac{\ell(S)}{E_j + \epsilon} \left| \begin{pmatrix} 0 & i\vec{\sigma} \\ -i\vec{\sigma} & 0 \end{pmatrix} \right| \frac{\ell(S')}{E_{j'} + \epsilon} \right\rangle \\
&= \gamma \left\langle \ell(S) \left| \frac{\vec{\sigma} \vec{k} \cdot \vec{\sigma} \sqrt{\epsilon}}{E_{j'} + \epsilon} + \frac{\vec{k} \cdot \vec{\sigma} \vec{\sigma} \sqrt{\epsilon}}{E_j + \epsilon} \right| \ell(S') \right\rangle, \tag{IIID23}
\end{aligned}$$

where

$$\gamma = \sqrt{\frac{\epsilon(E_j + \epsilon)(E_{j'} + \epsilon)}{4m_0 E_j E_{j'}}}. \tag{IIID24}$$

Using the relation

$$\sigma_j \sigma_k = \sigma_0 \delta_{jk} + i \epsilon_{jkl} \sigma_l, \tag{IIID25}$$

where σ_0 is the unit 2x2 matrix, ϵ_{jkl} is the completely antisymmetric tensor, and j, k and l are 1, 2, or 3, we find

$$\begin{aligned}
& \langle a^j(\vec{k}, S) | \vec{\chi} | a^{j'}(\vec{k}, S') \rangle \\
&= \frac{\gamma \sqrt{\epsilon} \langle \ell(S) | \vec{k}(2\epsilon + E_j + E_{j'}) + i \vec{k} \times \vec{\sigma} (E_j - E_{j'}) | \ell(S') \rangle}{(E_j + \epsilon)(E_{j'} + \epsilon)}. \tag{IIID26}
\end{aligned}$$

This result agrees with the one obtained by Wolff. For intraband transitions, it reduces to

$$\begin{aligned}
& \langle a^+(\vec{k}, S) | \vec{\chi} | a^+(\vec{k}, S') \rangle = - \langle a^-(\vec{k}, S) | \vec{\chi} | a^-(\vec{k}, S') \rangle \\
&= \frac{\vec{k} \cdot \vec{\epsilon}}{\hat{\epsilon} \sqrt{m_0}} \delta_{SS'}, \tag{IIID27a}
\end{aligned}$$

and for interband transitions we find

$$\begin{aligned}
& \langle a^+(\vec{k}, S) | \vec{\chi} | a^-(\vec{k}, S') \rangle = \langle a^-(\vec{k}, S') | \vec{\chi} | a^+(\vec{k}, S) \rangle^* \\
&= \frac{-\epsilon \langle \ell(S) | \vec{k} \epsilon + i \vec{k} \times \vec{\sigma} \hat{\epsilon} | \ell(S') \rangle}{\sqrt{m_0} \hat{\epsilon}^2 (\hat{\epsilon}^2 - \epsilon^2)}. \tag{IIID27b}
\end{aligned}$$

Let us first work out the intraband contribution to the conductivity, σ_{ii} .

Following the procedure of Eqs. IIIC24-27, we may show

$$\sigma_{\gamma\beta}^i = \sum_{j=1}^3 X_{\gamma}(j) X_{\beta}(j) \sigma_{oi}(j) \quad , \quad (\text{IIID28})$$

and

$$\begin{aligned} \sigma_{oi}(1) &= \sigma_{oi}(2) = \sigma_{oi}(3) \\ &= \frac{-2\tau e^2}{m_o(1-i\omega\tau)} \int \frac{\epsilon^2}{K} K^2 \frac{df(\hat{\epsilon})}{d\hat{\epsilon}} \\ &= \frac{-8\pi\tau e^2 c_k}{3m_o(1-i\omega\tau)} \int_0^{\infty} dK \frac{\epsilon^2 K^4}{\hat{\epsilon}^2} \frac{df(\hat{\epsilon})}{d\hat{\epsilon}} \quad . \end{aligned} \quad (\text{IIID29})$$

Once again c_k is the factor which takes into account the density of states involved in the conversion from the sum to the integral. Making the substitution

$$\epsilon K dK = \hat{\epsilon} d\hat{\epsilon} \quad , \quad (\text{IIID30})$$

we find

$$\sigma_{oi}(3) = \frac{-8\pi e^2 \tau c_k}{3m_o(1-i\omega\tau)} \int_{\epsilon}^{\infty} \frac{d\hat{\epsilon}(\hat{\epsilon}^2 - \epsilon^2)^{3/2}}{\sqrt{\hat{\epsilon}} \hat{\epsilon}} \frac{df(\hat{\epsilon})}{d\hat{\epsilon}} \quad , \quad (\text{IIID31})$$

and at $T=0$, where T is the absolute temperature, this becomes simply

$$\sigma_{ii}(3) = \frac{+8\pi e^2 \tau c_k}{3m_o(1-i\omega\tau)} \cdot \frac{(\hat{\epsilon}_f^2 - \epsilon^2)^{3/2}}{\sqrt{\hat{\epsilon}} \hat{\epsilon}} \quad . \quad (\text{IIID32})$$

To find c_k , we require

$$n = 2c_k \int d\vec{K} f(\hat{\epsilon}) = 8\pi c_k \int_0^{\infty} dK K^2 f(\epsilon) \quad , \quad (\text{IIID33})$$

where n is the electron density per ellipsoid. Using the substitution of Eq. IIID30, this becomes

$$n = 8\pi c_k \int_{\epsilon}^{\infty} \frac{\hat{\epsilon} d\hat{\epsilon}}{\epsilon} \sqrt{\frac{(\hat{\epsilon}^2 - \epsilon^2)}{\epsilon}} f(\hat{\epsilon}) \quad , \quad (\text{IIID34})$$

and at $T=0$, we find,

$$n = \frac{8\pi}{3} c_k \left(\frac{\hat{\epsilon}_f^2 - \epsilon^2}{\epsilon} \right)^{3/2} . \quad (\text{IIID35})$$

Therefore, at $T=0$,

$$\sigma_{oi}(3) = \frac{ne^2 \tau}{m_o(1-i\omega\tau)} \frac{\epsilon}{\hat{\epsilon}_f} . \quad (\text{IIID36})$$

Finally, we have

$$\sigma^i = \alpha \sigma_{oi}(3) . \quad (\text{IIID37})$$

At liquid helium temperatures, Eq. IIID36 is applicable. At higher temperatures, where $k_b T$ is of the order of $\hat{\epsilon}_f$, where k_b is Boltzmann's constant, (e.g. at 25°C $\hat{\epsilon}_f \approx k_b T$) Eqs. IIID31 and IIID34 must be evaluated by numerical means.

Let us now consider the contribution to the conductivity due to the interband transistions, σ^i , when $H=0$. It can also be shown in this case that the terms in Eq. IIIA25 involving $\langle \psi(z) | \chi(j) | \psi(z') \rangle \langle \psi(z') | \chi(l) | \psi(z) \rangle$ when $j \neq l$ contribute nothing to the total conductivity. Therefore, substituting IIID13, 18a and 27b into IIIA25, we may write

$$\sigma_{\gamma\beta}^t = \sum_j \sigma_{ot}(j) X_\gamma(j) X_\beta(j) , \quad (\text{IIID38})$$

and as before

$$\begin{aligned} \sigma_{ot}(1) &= \sigma_{ot}(2) = \sigma_{ot}(3) = \sigma_{ot}(j) \\ &= -e^2 \sum_{D, \vec{K}} g(D\hat{\epsilon}) \sum_{SS'} y_j(\vec{K}, D\hat{\epsilon}) , \end{aligned} \quad (\text{IIID39})$$

where

$$g(D\hat{\epsilon}) = \frac{[f(D\hat{\epsilon}) - f(-D\hat{\epsilon})] \epsilon^2}{2D\hat{\epsilon}(-i\omega + \frac{1}{\tau} + 2iD\hat{\epsilon}/\hbar) m_o \hat{\epsilon}^2 (\hat{\epsilon}^2 - \epsilon^2)} , \quad (\text{IIID40a})$$

$$y_j(\vec{K}, D\hat{E}) = \langle \ell(S) | \epsilon K_j + i(\vec{K} \times \vec{\sigma})_j D\hat{E} | \ell(S') \rangle \langle \ell(S') | \epsilon K_j - i(\vec{K} \times \vec{\sigma})_j D\hat{E} | \ell(S) \rangle, \quad (\text{IIID40b})$$

and $D = \pm 1$, depending on whether the initial state is in the valence or conduction band. Since we are summing over a complete set of spin states, and $\hat{E}$ is independent of spin, we may write

$$\begin{aligned} \sum_{SS'} y_j(\vec{K}, D\hat{E}) &= \sum_S \langle \ell(S) | (K_j \epsilon + i(\vec{K} \times \vec{\sigma})_j D\hat{E}) (K_j \epsilon - i(\vec{K} \times \vec{\sigma})_j D\hat{E}) | \ell(S) \rangle \\ &= \frac{1}{3} \sum_S \langle \ell(S) | K^2 \epsilon^2 + \hat{E}^2 (\vec{K} \times \vec{\sigma}) \cdot (\vec{K} \times \vec{\sigma}) | \ell(S) \rangle \\ &= \frac{1}{3} \sum_S \langle \ell(S) | K^2 (\epsilon^2 + 2\hat{E}^2) | \ell(S) \rangle = \frac{2}{3} K^2 (\epsilon^2 + 2\hat{E}^2). \end{aligned} \quad (\text{IIID41})$$

We may now write Eq. IIID39 as

$$\begin{aligned} \sigma_{\text{ot}}(j) &= \frac{2}{3} e^2 c_k \sum_D \int d\vec{K} g(D\hat{E}) K^2 (\epsilon^2 + 2\hat{E}^2) \\ &= \frac{8\pi e^2 c_k}{3m_0} \int_{\epsilon}^{\hat{E}_u} d\hat{E} \frac{\hat{E}^2 - \epsilon^2}{\epsilon} \frac{(\epsilon^2 + 2\hat{E}^2) (\frac{1}{\tau} - i\omega) (f[-\hat{E}] - f[\hat{E}])}{\hat{E}^2 ([\frac{1}{\tau} - i\omega]^2 + 4\hat{E}^2/\hbar^2)}. \end{aligned} \quad (\text{IIID42})$$

The upper limit $\hat{E}_u$, limits the integral to energies low enough so that the Wolff Hamiltonian of Eq. IIID10 is adequate. It will shortly be shown that our results are essentially independent of $\hat{E}_u$, as long as it is sufficiently large.

At $T=0$, we may do the integral of Eq. IIID42 and evaluate c_k to find

$$\begin{aligned} \sigma_{\text{ot}}(j) &= \frac{ne^2 \hbar}{4\epsilon m_0 (\hat{E}_f^2/\epsilon^2 - 1)^{3/2}} \left[\left(\frac{2}{\beta^2} - 1 \right) \beta^{2+4} \ln \left\{ \frac{x-x_+}{x-x_-} \right\} \right. \\ &\quad \left. + \frac{8}{(1+x)\beta} + \beta \ln(x) \right] \bigg|_{x(\hat{E}_f/\epsilon)}^{x(\hat{E}_u/\epsilon)}, \end{aligned} \quad (\text{IIID43})$$

where

$$x(u) = 2u^2 - 1 + 2u\sqrt{u^2 - 1} \quad , \quad (\text{IIID44})$$

$$x_{\pm} = -\frac{\beta^2 + 2}{2} \pm \frac{1}{2}\beta\sqrt{\beta^2 + 4} \quad , \quad (\text{IIID45})$$

and

$$\beta = \left(\frac{1}{\tau} - i\omega\right)\hbar/\epsilon \quad , \quad (\text{IIID46})$$

and finally, the complete contribution to the conductivity of the tightly coupled valence and conduction bands at L is

$$\vec{\sigma} = \vec{\alpha}(\sigma_{oi}(3) + \sigma_{ot}(3)) \quad . \quad (\text{IIID47})$$

Let us consider this result in some detail. In Fig. 13, we plot the real and imaginary parts of σ_{xx} using parameters which have been found to give a good fit to the zero field transmission experiments of Boyle and Brailsford⁽⁷⁰⁾ (see Fig. 16), as is discussed in Section IIIF.

The first term in Eq. IIID43 is responsible for the structure observed in Fig. 13 near the interband transition frequency. As long as $\hat{\epsilon}_u \gg \hbar\omega$, which is normally the case, the value of this term is insensitive to the value we choose for $\hat{\epsilon}_u$. The second term in Eq. IIID43 has the frequency dependence of an ordinary free electron term, as does $\sigma_{oi}(3)$, and is also insensitive to the value of $\hat{\epsilon}_u$, as long as $\hat{\epsilon}_u \gg \hat{\epsilon}_f$; a condition which is always satisfied.

The final term has the frequency dependence of a contribution from the dielectric constant, and displays a logarithmic dependence on the value of $\hat{\epsilon}_u$. This causes no difficulty, however, because varying $\hat{\epsilon}_u$ merely moves the arbitrary dividing line between the contribution to the conductivity from those transitions included explicitly in the integral of Eq. IIID43 and those included implicitly in the field and frequency

independent "core" dielectric constant tensor, ϵ_c , which was introduced in Section IIIA. Thus we see that the apparent logarithmic divergence of the integral of Eq. IIID43 actually causes no difficulty in the calculation.

Let us now evaluate the conductivity in the presence of a magnetic field. We must first solve the secular equation

$$H_0 F = EF, \quad (\text{IIID48a})$$

where H_0 is the 4x4 Wolff Hamiltonian of Eq. IIID18b, and F is its four component eigenfunction. It is clear that the solution of IIID48a would be considerably simplified if we could choose the vectors $\vec{X}(j)$ such that $b_1 = b_2 = 0$, and $b_3 > 0$, where by analogy with Eq. IIIC32-34 we would define b_l by the equation

$$\sum_{m,j} [P_m, P_j] \epsilon_{mj l} = \sum_{m,j} i \vec{X}(m) \times \vec{X}(j) \cdot \vec{H} \frac{e \hbar}{m_0 c} \epsilon_{mj l} \equiv i b_l. \quad (\text{IIID48b})$$

This choice of the vectors $\vec{X}(j)$ would greatly simplify the representation of the operators P_j . However, as we have used them, the vectors $\vec{X}(j)$ are not arbitrary, but are fixed by our choice of basis. Therefore, let us first consider a set of three real vectors, $\vec{W}(j)$, which are arbitrary, subject only to the condition

$$\alpha_{\beta\gamma} = \sum_{j=1}^3 \vec{W}_{\beta}(j) \vec{W}_{\gamma}(j). \quad (\text{IIID49})$$

One can always then find a linear transformation, R_{ij} , such that

$$\vec{W}(i) = R_{ij} \vec{X}(j). \quad (\text{IIID50})$$

It can be shown that R_{ij} has the very useful property that

$$\sum_j R_{ji} R_{jl} = \delta_{il}. \quad (\text{IIID51})$$

by noting

$$\begin{aligned} \sum_j X_\beta(j) X_\gamma(j) &= \alpha_{\beta\gamma} = \sum_j W_\beta(j) W_\gamma(j) \\ &= \sum_{j, \ell, m} X_\beta(\ell) R_{j\ell} R_{jm} X_\gamma(m) \quad . \end{aligned} \quad (\text{IIID52})$$

Defining

$$P_j \equiv \vec{\pi} \cdot \vec{W}(j) / \sqrt{m_0} = R_{ji} P_i \quad , \quad (\text{IIID53a})$$

$$\sum_{m, j} [P'_m, P'_j] \epsilon_{ij\ell} = \sum_{m, j} i \vec{W}(m) \times \vec{W}(j) \cdot \vec{H} \frac{e\hbar}{m_0 c} \epsilon_{mj\ell} \equiv b'_\ell \quad , \quad (\text{IIID53b})$$

and

$$\sigma'_j \equiv R_{ji} \sigma_i \quad , \quad (\text{IIID54})$$

we can use Eq. IIID51 to show

$$H_0 = \begin{pmatrix} \epsilon & i\sqrt{\epsilon} \vec{P}' \cdot \vec{\sigma}' \\ -i\sqrt{\epsilon} \vec{P}' \cdot \vec{\sigma}' & -\epsilon \end{pmatrix} \quad , \quad (\text{IIID55})$$

and

$$\vec{V}_0 = \sum_j \vec{W}(j) \chi'(j) \quad , \quad (\text{IIID56})$$

where

$$\chi'(j) = \sqrt{\frac{\epsilon}{m_0}} \begin{pmatrix} 0 & i\sigma'_j \\ -i\sigma'_j & 0 \end{pmatrix} \quad . \quad (\text{IIID57})$$

We can then choose $\vec{W}(3)$ parallel to $\vec{H}$ to simplify the representation of the operators P'_j by making $b'_1 = b'_2 = 0$, and b'_3 positive. We may also perform a unitary transformation on the basis states such that in the new basis,

$$\sigma'_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad (\text{IIID58a})$$

$$\sigma'_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad (\text{IIID58b})$$

and

$$\sigma'_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad . \quad (\text{IIID58c})$$

Let us assume that this has been done and drop the primes.

The simplest way to solve Eq. IIID48a is now to write

$$F = C_n \begin{pmatrix} x_u \\ x_\ell \end{pmatrix} \quad , \quad (\text{IIID59})$$

where x_u and x_ℓ are each two component functions, and C_n is a normalizing factor; and then to rewrite the secular equation in the form of two equations:

$$(\epsilon - E)x_u + i\sqrt{\epsilon} \vec{P} \cdot \vec{\sigma} x_\ell = 0 \quad , \quad (\text{IIID60})$$

and

$$-i\sqrt{\epsilon} \vec{P} \cdot \vec{\sigma} x_u - (E + \epsilon)x_\ell = 0 \quad . \quad (\text{IIID61})$$

Solving Eq. IIID61 for x_ℓ we find

$$x_\ell = -i \frac{\sqrt{\epsilon} \vec{P} \cdot \vec{\sigma} x_u}{E + \epsilon} \quad , \quad (\text{IIID62})$$

and substituting this in IIID60 we find

$$\begin{aligned} E^2 x_u &= (\epsilon^2 + [\vec{P} \cdot \vec{\sigma}]^2 \epsilon) x_u = (\epsilon^2 + [P^2 + i \vec{P} \times \vec{P} \cdot \vec{\sigma}] \epsilon) x_u \\ &= (\epsilon^2 + [P^2 - \vec{b} \cdot \vec{\sigma}] \epsilon) x_u \quad . \end{aligned} \quad (\text{IIID63})$$

The eigenvalues of this equation are

$$E_{\pm}(n, K_3, S) = \pm \hat{E}(n, K_3, S) \quad , \quad (\text{IIID64})$$

where + and - signs refer to the conduction and valence bands, respectively,

and

$$\begin{aligned} \hat{E}(n, K_3, S) &= \sqrt{\epsilon^2 + \epsilon b_3(2n+1-S) + \epsilon K_3^2} \\ &= \sqrt{\frac{E^2}{4} + \frac{E}{2} (\beta^* H[2n+1-S] + \frac{h^2 k_H^2}{m_H m_O})} \quad , \end{aligned} \quad (\text{IIID65})$$

where we have used the representation of the operators P_j presented in Eqs. IIIC42 and 44-46 and the Eqs. IIIC63-65:

$$H\beta^* = b_3 = \frac{|e|\hbar(\vec{H} \cdot \vec{m}^{**} \cdot \vec{H})^{1/2}}{m_0 c |\vec{m}^{**}|^{1/2}}, \quad (\text{IIIC63})$$

$$K_3^2 = k_H^2 / m_H m_0, \quad (\text{IIIC64})$$

and

$$m_H = \vec{H} \cdot \vec{m}^{**} \cdot \vec{H} / H^2, \quad (\text{IIIC65})$$

where $\vec{m}^{**} = (\vec{g})^{-1}$ is the effective mass tensor at the bottom of the band, and $\hbar k_H$ is the crystalline momentum parallel to the magnetic field.

The two eigenfunctions of Eq. IID63 are

$$x_u(n, K_3, S) = \phi(n, K_3) \ell(S), \quad (\text{IID66})$$

where $\phi(n, K_3)$ is a harmonic oscillator function and $\ell(S)$ is a spinor:

$$\ell(1) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (\text{IID67a})$$

and

$$\ell(-1) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (\text{IID67b})$$

The corresponding four component eigenfunctions of the secular equation

IID48, are then found to be

$$F_{\pm}(n, K_3, S) = C_n \frac{x_u(n, K_3, S) \mp i \sqrt{E} \vec{P} \cdot \vec{\sigma} x_u(n, K_3, S)}{(n, K_3, S) + E}, \quad (\text{IID68})$$

where the normalization factor, C_n is

$$C_n = \sqrt{\frac{E+E}{2E}}. \quad (\text{IID69})$$

One may now evaluate the matrix element of $\vec{\chi}$, which is related to the velocity operator by Eq. IID56, between these eigenstates of H_0 to find

$$\langle F | \vec{\chi} | F' \rangle = \sqrt{E} \gamma \frac{\langle x_u | \vec{P}(2E+E+E') + i \vec{P} \times \vec{\sigma} (E-E') | x'_u \rangle}{(E+E)(E'+E)}, \quad (\text{IID70})$$

where the expression for γ is again given by Eq. IIID24. This equation also agrees with the one derived by Wolff.

We can once again show that Eq. IIIC53 is true, and using the equation

$$i \int \epsilon_{jkl} \vec{W}(j) P_k \sigma_l = \vec{W}(+) (P_3 \sigma_- - P_- \sigma_3) + \vec{W}(-) (P_+ \sigma_3 - P_3 \sigma_+) + \vec{W}(3) (P_- \sigma_+ - P_+ \sigma_-) , \quad (\text{IIID71})$$

we may show

$$\chi(-) = \epsilon \gamma \frac{\langle x_u | P_- (2\epsilon + E + E') + (E - E') (P_3 \sigma_- - \sigma_3 P_-) | x'_u \rangle}{(E + \epsilon) (E' + \epsilon)} , \quad (\text{IIID72})$$

$$\chi(+) = \epsilon \gamma \frac{\langle x_u | P_+ (2\epsilon + E + E') + (E - E') (P_+ \sigma_3 - P_3 \sigma_+) | x'_u \rangle}{(E + \epsilon) (E' + \epsilon)} , \quad (\text{IIID73})$$

and

$$\chi(3) = \sqrt{\epsilon} \gamma \frac{\langle x_u | P_3 (2\epsilon + E + E') + (E - E') (P_- \sigma_+ - P_+ \sigma_-) | x'_u \rangle}{(E + \epsilon) (E' + \epsilon)} . \quad (\text{IIID74})$$

We could now calculate the conductivity using Eq. IIIC51, substituting the proper expressions for E , $\chi(+)$ and $\chi(-)$ in Eq. IIIC52 for σ_{+-} , and, in a similar manner, calculating σ_{-+} and σ_{33} .

However, we do not require σ_{33} in our calculation of the optical conductivity, since our experiments are done in the geometry where $\vec{E} \perp \vec{H}$. Since $\vec{H} \parallel \vec{W}(3)$, we see $\vec{E} \cdot \vec{W}(3) = 0$, and therefore σ_{33} makes no contribution to the current. Furthermore, we can considerably simplify the expressions for σ_{+-} and σ_{-+} and relate one to the other, which greatly simplifies the actual evaluation of the formulas. Using the easily proven relation

$$\langle F | \chi(+) | F' \rangle = \langle F' | \chi(-) | F \rangle , \quad (\text{IIID75})$$

we may write a combined equation for both σ_{+-} and σ_{-+} ,

$$\sigma_M = -e^2 \int \frac{(\bar{f} - f') |\langle F | \chi(+) | F' \rangle|^2}{(E - E') (-i\omega + \frac{1}{\tau} + \frac{i}{\hbar} M[E - E'])} , \quad (\text{IIID76})$$

where σ_M corresponds to σ_+ or σ_- when $M = +1$ or -1 , respectively. The sum is over all coupled eigenstates, F and F' . The equation includes both inter and intra-band contributions to the conductivity. Therefore we need evaluate only one type of matrix element to calculate the conductivity.

It is convenient to divide σ_M into two parts: a) that part, σ_M^C , which comes from terms where F and F' have the same spin (spin conserving contribution); and b) that part, σ_M^F , which comes from terms where F and F' have opposite spins (spin flipping contribution). Since for a spin flipping term, $\chi(+)$ only involves P_3 and σ_+ , (see Eq. IIID73) S must be $+1$, $S' = -1$, and $n = n'$, so we may write

$$\sigma_M^F = - \frac{e^2 \epsilon^2 c_k}{2m_0} \sum_{D, D', n} \int_0^{K_u} dK_3 \frac{(f-f')(E-E')K_3^2}{EE'(E+\epsilon)(E'+\epsilon)(-i\omega + \frac{1}{\tau} + \frac{i}{\hbar} M[E-E'])} , \quad (\text{IIID77})$$

where K_u is that value of K_3 which corresponds to $\hat{\epsilon}_u$ (see Eq. IIID65), and D and D' are the band indices for E and E' , respectively. To evaluate the normalizing factor, c_k , we require

$$n_e = c_k \sum_{S, n} \int_0^\infty dK_3 f(\hat{\epsilon}) , \quad (\text{IIID78})$$

where n_e is the density of electrons per ellipsoid. At $T=0$, this becomes

$$n_e = \frac{c_k}{\sqrt{\epsilon}} \sum_{S, n} R_e \{ (\hat{\epsilon}_f^2 - \epsilon^2 - \epsilon b[2n+1-S])^{1/2} \} . \quad (\text{IIID79})$$

For the spin conserving contribution, $\chi(+)$ only involves P_+ and σ_3 so that $n' = n+1$ and $S = S'$ so we may write

$$\sigma_M^C = \frac{-e^2 \epsilon^2 c_k}{4m_0} \sum_{D, D', n, S} \int_0^{K_u} dK_3 \frac{(f-f')(n+1)b_3(2\epsilon+E+E'+S[E-E'])^2}{EE'(E+\epsilon)(E'+\epsilon)(E-E')(-i\omega + \frac{1}{\tau} + \frac{i}{\hbar} M[E-E'])} \quad (\text{IIID80})$$

These expressions cannot be evaluated analytically, and have been integrated and summed by numerical techniques. These techniques are discussed in Appendix D. Before we work out these equations in detail, however, let us first consider the small terms of the Baraff Hamiltonian, which we have completely neglected up to now, and see what sort of modifications they make in the equations derived so far. This will be done in Section IIIE.

SECTION IIIE

THE FULL BARAFF HAMILTONIAN

In this section we will consider H , the full Baraff Hamiltonian⁽³⁹⁾ of Eq. IIID9. Let us first make some introductory remarks about the band structure predicted by this Hamiltonian with the magnetic field equal to zero. In that case, it is simple to find E_+ and E_- , the exact eigenvalues of H corresponding to the conduction and valence bands, respectively. One finds

$$E_{\pm} = \pm \sqrt{\epsilon^2 + \epsilon \vec{k} \cdot \frac{(\vec{\beta} + \vec{\alpha}^w)}{m_0} \cdot \vec{k} \hbar^2 + \frac{(\vec{k} \cdot \vec{\beta} \cdot \vec{k})^2}{2m_0} \hbar^4}, \quad (\text{IIIE1})$$

where we have used the relation

$$\vec{\beta} \equiv \vec{\beta}^c = -\vec{\beta}^v, \quad (\text{IIIE2a})$$

which follows from Eq. IIIC7; and $\vec{\alpha}^w$ is a tensor, analogous to the one defined by Wolff⁽¹⁰⁾ in Eq. IIID16, so that

$$\alpha_{\gamma\nu}^w = \sum_j X_{\gamma}(j) X_{\nu}(j). \quad (\text{IIIE2b})$$

Note that now $\vec{\alpha}^w$ and $\vec{\beta}$ are merely two tensors to be experimentally evaluated; $\vec{\alpha}^w$ is not directly related to the curvature at the bottom of the band, since both $\vec{\beta}$ and $\vec{\alpha}^w$ contribute to the curvature here.

The nature of the dispersion relation described by Eq. IIIE1 depends upon the relative magnitudes of the quantities ϵ , $\vec{\alpha}^w$, and $\vec{\beta}$. First of all, it is well known that ϵ is very small,⁽³⁾ being only a small fraction of the Fermi energy. Secondly, it has also been firmly established that the Lax model accurately describes the dispersion relation for $\vec{k}$ perpendicular to $\vec{B}$,⁽⁵⁴⁾

where $\vec{B}$ is a unit vector in the Brillouin zone pointing along the long axis of the carrier pocket. This implies that $\vec{\lambda}_\perp \cdot \vec{\alpha}^w \cdot \vec{\lambda}_\perp \gg \vec{\lambda}_\perp \cdot \vec{\beta} \cdot \vec{\lambda}_\perp$, where $\vec{\lambda}_\perp$ is a unit vector in the Brillouin zone perpendicular to $\vec{B}$. In addition, the high band curvature in these directions implies that $\vec{\lambda} \cdot \vec{\alpha}^w \cdot \vec{\lambda} \gg 1$.

Aside from the inequalities above, we actually know very little about the magnitude of the tensor $\vec{\beta}$. It is clear, however, that no matter how small $\vec{\beta}$ is, at sufficiently high energies the $(\vec{k} \cdot \vec{\beta} \cdot \vec{k})^2$ term inside the square root of Eq. III E1 will dominate and the Lax model will break down. At these high energies, the bands will behave like simple parabolic bands with a reciprocal effective mass tensor of $\vec{\beta}$, and since, at these high energies, all of the strongly interacting bands will be far away in energy, it would be reasonable to assume that $\vec{\beta}$ is of the order of unity. It should be emphasized, however, that this estimate is extremely rough, and we would not be surprised to find that the magnitude of $\vec{\beta}$ in a given direction is a factor of ten or more either side of unity. It should also be noted that at intermediate energies, where the Lax model still holds, there will be a band curvature minimum, where the band curvature corresponds to a reciprocal effective mass tensor much less than either $\vec{\alpha}^w$ or $\vec{\beta}$. Therefore, in terms of the dispersion relation of Eq. III E1 we can now understand how the Lax model can indeed apply in a region of very low band curvature.

Although the nature of the dispersion relation for $\vec{k}$ perpendicular to $\vec{B}$ is well known, there has been a considerable amount of controversy^(54,71-72) about the nature of the bands when $\vec{k}$ is parallel to $\vec{B}$. In the Lax model,⁽³⁵⁾ we would assume that at the energies of interest, it is still possible to make the approximation $\vec{B} \cdot \vec{\beta} \cdot \vec{B} = 0$, thereby obtaining an ellipsoidal Fermi surface.

Cohen,⁽⁵⁴⁾ however, noted that the elongation of the carrier pockets in the $\vec{B}$ direction indicated that the conduction and valence bands were not strongly interacting in that direction. He therefore assumed that $\vec{B} \cdot \vec{\alpha}^w \cdot \vec{B} = 0$, which requires that the Fermi surface have a decidedly non-ellipsoidal nature. Recent experiments,⁽⁴⁰⁾ however, have shown that the Fermi surface is almost exactly ellipsoidal, so we therefore conclude that the assumption of Cohen is incorrect,⁽⁷³⁾ and that $\vec{B} \cdot \vec{\alpha}^w \cdot \vec{B}$ is not zero, but is actually considerably larger than $\vec{B} \cdot \vec{\beta} \cdot \vec{B}$.

Unfortunately it is very difficult to obtain more information about the magnitude of $\vec{B} \cdot \vec{\beta} \cdot \vec{B}$. Almost certainly, however, it is not as large as one, since in that case we would expect there to be large deviations from the Lax model at the Fermi surface, and the deviations which do exist are known to be small. We will therefore assume that $\vec{B} \cdot \vec{\beta} \cdot \vec{B} \leq 1/2$, which is not an unreasonably small value for this quantity,* and yields a band structure which deviates only slightly from the Lax model at the Fermi surface. With this assumption we find that $\vec{B} \cdot \vec{\alpha}^w \cdot \vec{B}$ is about 4, so that $\vec{B} \cdot \vec{\alpha}^w \cdot \vec{B} \gg \vec{B} \cdot \vec{\beta} \cdot \vec{B}$ and we may therefore treat the Baraff interaction by perturbation theory when solving the more difficult magnetic field problem.

We could, at this point, attempt to calculate the zero field contribution to the conductivity due to the conduction and valence bands using the technique of Section IIID. We would, however, find it very difficult to do so due to the complicated form of the dispersion relation, and the even more complicated

*The essential motivation for the Cohen model was that the Lax model requires $\vec{B} \cdot \vec{\beta} \cdot \vec{B} = 0$, which is an unreasonably small value for this parameter.

form of the expressions for the necessary matrix elements of the effective mass velocity operator. Since β is small, and the zero field optical data are not sensitive to the fine details of the band structure, we will go no further with the zero field conductivity calculation.

Experiments performed in the presence of a magnetic field, however, are far more sensitive to the fine details of the band structure. For example, the splittings observed in the giant quantum oscillations in the ultrasonic magnetoattenuation^(38,98) are due to the small additional terms in the Baraff Hamiltonian, which split the Landau level degeneracies predicted by the Wolff Hamiltonian. We therefore will carefully consider the effects of the additional terms in the Baraff Hamiltonian on the Landau level structure.

In the presence of a magnetic field, the Baraff Hamiltonian cannot be exactly diagonalized, and we will therefore first calculate the Landau level energies to the first order in perturbation theory, writing

$$H = H_0 + H_p \quad (\text{IIIE3})$$

where H_0 is the Wolff Hamiltonian of Eq. IID10, and H_p , the perturbation Hamiltonian,* is

$$H_p = \sum_{j=1}^3 \begin{pmatrix} \vec{\pi} \cdot \frac{\vec{\omega}^c}{2m_0} \cdot \vec{\pi} + \sigma_j \mathcal{A}_j^c & 0 \\ 0 & \vec{\pi} \cdot \frac{\vec{\omega}^v}{2m_0} \cdot \vec{\pi} + \sigma_j \mathcal{A}_j^v \end{pmatrix}, \quad (\text{IIIE4})$$

* We do not set $\vec{\omega}^c = -\vec{\omega}^v$ because at this point we are trying to derive the expressions required to justify this equation.

This problem was first considered by Baraff, who derived a rather complicated expression for the energy when $k_H = 0$. Using the results of our magnetoreflexion experiments, we have been able to simplify his expressions, and using these simplifications, we have been able to extend his results to include the case where $k_H \neq 0$. In the first part of this section, we will explain how this was done, and present our more complete expressions for the Landau level energies. These equations will involve quantities which depend on the orientation of the magnetic field, but not on its magnitude. We will find the transformation properties of these quantities in the second part of this section. At the end of the second part of this section, we will also bring together all of the equations required for calculating the Landau level energies with the Baraff interaction⁽³⁹⁾ taken into account. We hope that these expressions will be of use to investigators requiring accurate expressions for these energies.

Finally, in the third part of this section, we will find expressions for the velocity matrix elements between the eigenfunctions of the full Baraff Hamiltonian. We will require these expressions when we consider the effects of the Baraff interaction on the magnetoreflexivity.

THE LANDAU LEVEL ENERGIES

To simplify our calculation, let us first write H_p using the quantities P_j defined in Eq. IIID17a in place of $\vec{\pi}$; and treat the quantities P_j , σ_j , $\mathcal{L}_j^c$ and $\mathcal{X}_j^v$ as vectors in a transformed space.⁽¹⁰⁾ Defining $\hat{B}_{lm}^c$, a tensor in the transformed space, by the equation

$$\beta_{\gamma\Delta}^c = \sum_{l,m} X_\gamma(l) B_{lm}^c X_\Delta(m) , \quad (\text{IIIE5})$$

and using a similar relation to define $\hat{B}_{lm}^v$, we may write

$$H_P = \begin{pmatrix} \vec{p} \cdot \frac{\overleftrightarrow{B}^c}{2} \cdot \vec{p} + \mathcal{L}^c \cdot \vec{\sigma} & 0 \\ 0 & \vec{p} \cdot \frac{\overleftrightarrow{B}^v}{2} \cdot \vec{p} + \mathcal{L}^v \cdot \vec{\sigma} \end{pmatrix}. \quad (\text{III E6})$$

As we did in Section IIID, Eqs. IIID49-55, we will now introduce the arbitrary set of real space vectors, $\vec{W}(j)$, and the quantities P_j' and σ_j' which depend on our choice of these vectors. We then find

$$H_P = \begin{pmatrix} \vec{p}' \cdot \frac{\overleftrightarrow{B}^c}{2} \cdot \vec{p}' + \vec{p}' + \vec{L}^c \cdot \vec{\sigma}' & \\ 0 & \vec{p}' \cdot \frac{\overleftrightarrow{B}^v}{2} \cdot \vec{p}' + \vec{p}' + \vec{L}^v \cdot \vec{\sigma}' \end{pmatrix}, \quad (\text{III E7})$$

where

$$\overleftrightarrow{B}^c \equiv \overleftrightarrow{R} \cdot \overleftrightarrow{B}^c \cdot \overleftrightarrow{R}^T, \quad (\text{III E8a})$$

and

$$\vec{L}^c \equiv \overleftrightarrow{R} \cdot \vec{L}^c, \quad (\text{III E8b})$$

and we use similar relations to define $\overleftrightarrow{B}^v$ and $\vec{L}^v$. The symbol $\overleftrightarrow{R}^T$ means the transpose of matrix $\overleftrightarrow{R}$. Once again we will choose the vectors, $\vec{W}(j)$ such that $b_1' = b_2' = 0$ and $b_3' > 0$, and then perform a unitary transformation on the basis so that the matrices σ_j' have the simple form of Eq. IIID58. Assuming this

has been done; we will drop the primes from b'_j , P'_j and σ'_j for the remainder of this section. It should be pointed out that now the basis depends on the orientation of the magnetic field so that the transformation properties of $\vec{L}^c$, $\vec{L}^v$, $\vec{B}^c$ and $\vec{B}^v$ will be quite complicated. We will explore these transformation properties in the second part of this section.

Let us now consider the effects of the perturbation Hamiltonian, H_p , on the Landau levels which are degenerate in the Lax model. First of all, we will find it convenient to label the eigenvalues and eigenfunctions of H_0 , which we will call E_0 and F_0 , respectively, with the quantum numbers J and S , rather than n and S , where

$$J = 2n+1-S, \quad (\text{IIIE9})$$

because E_0 then only depends on K_3 , J , and D (the band index) and not on S . From Eq. IIIE9, J must be an even integer, and we see that we may easily describe the doubly degenerate Landau levels given by the Wolff Hamiltonian, as the $J \neq 0$ Landau levels. (See Section IIC for a more detailed discussion of these points).

To calculate the effects of H_p on the $J \neq 0$ Landau levels, we will now employ degenerate first order perturbation theory.⁽³⁹⁾ We therefore require the diagonal matrix elements of H_p , and also the matrix elements between the degenerate J, S and $J, -S$ Landau levels. These matrix elements may be written as

$$\langle F_0(D, K_3, J, S) | H_p | F_0(D, K_3, J, S') \rangle$$

$$\begin{aligned}
&= \frac{E_0 + \epsilon}{2E_0} \left\langle \begin{array}{c} x_u \\ \frac{-i\sqrt{\epsilon} \vec{P} \cdot \vec{\sigma} x_u}{E_0 + \epsilon} \end{array} \right| \begin{array}{cc} \vec{P} \cdot \frac{\vec{B}^c}{2} \cdot \vec{P} + \vec{L}^c \cdot \vec{\sigma} & 0 \\ 0 & \vec{P} \cdot \frac{\vec{B}^v}{2} \cdot \vec{P} + \vec{L}^v \cdot \vec{\sigma} \end{array} \left| \begin{array}{c} x'_u \\ \frac{-i\sqrt{\epsilon} \vec{P} \cdot \vec{\sigma} x'_u}{E_0 + \epsilon} \end{array} \right\rangle \\
&= \frac{E_0 + \epsilon}{2E_0} \left\{ \langle x_u | \vec{P} \cdot \frac{\vec{B}^c}{2} \cdot \vec{P} + \vec{L}^c \cdot \vec{\sigma} | x'_u \rangle + \epsilon \frac{\langle x_u | \vec{P} \cdot \vec{\sigma} (\vec{P} \cdot \frac{\vec{B}^v}{2} \cdot \vec{P} + \vec{L}^v \cdot \vec{\sigma}) \vec{P} \cdot \vec{\sigma} | x'_u \rangle}{(E_0 + \epsilon)^2} \right\}.
\end{aligned}
\tag{IIIE10}$$

This expression may be greatly simplified by noting that, of the complicated operators involved, we only require that part which couples states of the same J , since states of different J cannot be degenerate.⁽³⁹⁾ Considering the first term of Eq. IIIE10, for example, calling ξ_c that part of $\vec{L}^c \cdot \vec{\sigma}$ diagonal in J , we see

$$\xi_c = L_3^c \sigma_3, \tag{IIIE11}$$

since the quantities, L_j^c and L_j^v are merely C numbers. The corresponding part of $\vec{P} \cdot \frac{\vec{B}^c}{2} \cdot \vec{P}$ we will call Λ_c and may write

$$\Lambda_c = P^2 B_a^c + P_3^2 B_b^c, \tag{IIIE12}$$

where

$$B_a^c = (B_{11}^c + B_{22}^c)/4, \tag{IIIE13a}$$

and

$$B_b^c \equiv (2B_{33}^c - B_{11}^c - B_{22}^c)/4 \quad , \quad (\text{III E13b})$$

We will now find the corresponding operators Λ_v and ξ_v for the second term of Eq. III E10.

Noting that since $\vec{P} \cdot \vec{\sigma}$ is diagonal in J, so that we only require that part of $\vec{L}^v \cdot \vec{\sigma}$ which is diagonal in J, we may write

$$\xi_v = \vec{P} \cdot \vec{\sigma} L_3^v \sigma_3 \vec{P} \cdot \vec{\sigma} \quad , \quad (\text{III E14})$$

It may then be shown by straightforward operator manipulation that

$$\xi_v = L_3^v [2P_3 \vec{P} \cdot \vec{\sigma} - \sigma_3 (\vec{P} \cdot \vec{\sigma})^2] \quad , \quad (\text{III E15})$$

It is more difficult to work out Λ_v . Once again noting that since $\vec{P} \cdot \vec{\sigma}$ is diagonal in J, we only require that part of $\vec{P} \cdot \vec{B}^v \cdot \vec{P}/2$ which is diagonal in J, we may write

$$\Lambda_v = \vec{P} \cdot \vec{\sigma} (B_a^v P^2 + B_b^v P_3^2) \vec{P} \cdot \vec{\sigma} \quad , \quad (\text{III E16})$$

It may be shown that

$$(\vec{P} \cdot \vec{\sigma}) P^2 (\vec{P} \cdot \vec{\sigma}) = (P^2 - 2\vec{b} \cdot \vec{\sigma}) (\vec{P} \cdot \vec{\sigma})^2 + 2\vec{P} \cdot \vec{\sigma} \vec{P} \cdot \vec{b} \quad , \quad (\text{III E17})$$

so that

$$\Lambda_v = B_a^v [(P^2 - 2b_3 \sigma_3) (\vec{P} \cdot \vec{\sigma})^2 + 2P_3 b_3 \vec{P} \cdot \vec{\sigma}] + B_b^v P_3^2 (\vec{P} \cdot \vec{\sigma})^2 \quad , \quad (\text{III E18})$$

Substituting the relation

$$E_0^2 - \epsilon^2 = \epsilon (\vec{P} \cdot \vec{\sigma})^2 \quad , \quad (\text{III E19})$$

into Eq. IIIE10, we find

$$\begin{aligned}
\langle F_o | H_p | F_o' \rangle &= \frac{E_o + \epsilon}{2E_o} \langle x_u | B_a^c P^2 + B_b^c P_3^2 + L_3^c \sigma_3 | x_u' \rangle \\
&+ \frac{E_o - \epsilon}{2E_o} \langle x_u | B_a^v (P^2 - 2b_3 \sigma_3) + B_b^v P_3^2 - L_3^v \sigma_3 | x_u' \rangle \\
&+ \frac{\epsilon (B_a^v b_3 + L_3^v)}{E_o (E_o + \epsilon)} \langle x_u | P_3 \vec{P} \cdot \vec{\sigma} | x_u' \rangle ,
\end{aligned} \tag{IIIE20}$$

We now may evaluate the matrix elements of H_p between the degenerate eigenstates of H_o . The matrix elements between the two degenerate solutions of opposite spin are

$$\begin{aligned}
\langle F_o(S) | H_p | F_o(-S) \rangle &= \frac{\epsilon v_v H K_3}{E_o (E_o + \epsilon)} \langle x_u(S) | \vec{P} \cdot \vec{\sigma} | x_u(-S) \rangle \\
&= \langle F_o(-S) | H_p | F_o(S) \rangle = \frac{\epsilon v_v H K_3}{E_o (E_o + \epsilon)} \sqrt{b_3 J} ,
\end{aligned} \tag{IIIE21}$$

where we have defined

$$v_i \equiv (B_a^i b_3 + L_3^i) / H , \tag{IIIE22}$$

where $i = v$ or c . Since both b_3 (Eq. IIIC63) and L_3^v (Eqs. IIID6 and IIIE8b) were defined to have a linear magnetic field dependence, the quantity v_i is independent of the magnitude of the magnetic field, but does depend on its direction.

The diagonal matrix element of H_p diagonal in S can be written, using Eqs. IIIIE13a and b,

$$\begin{aligned}
 \langle F_o | H_p | F_o \rangle &= \frac{E_o + \epsilon}{2E_o} (B_{a3}^c b_3 J + \frac{1}{2} B_{33}^c K_3^2 + H v_c S) \\
 &+ \frac{E_o - \epsilon}{2E_o} (B_{a3}^v b_3 J + \frac{1}{2} B_{33}^v K_3^2 - H v_v S) \\
 &+ \frac{H v_v S \epsilon K_3^2}{E_o (E_o + \epsilon)} \quad . \quad (IIIIE23)
 \end{aligned}$$

We have now found all the necessary matrix elements of H_p between the degenerate eigenfunctions of H_o , and may proceed to evaluate the corresponding eigenvalues, E , and eigenfunctions, F , of the Baraff Hamiltonian, H , to first order in perturbation theory.

Let us first determine the energies at $K_3 = 0$ (i.e. $k_H = 0$). These energies determine the fields at which there will be a peak in the conductivity due to the associated peak in the joint density of states. When $K_3 = 0$, the interaction term of Eq. IIIIE21 is zero, so that F_o is an approximate eigenfunction of H as well as of H_o , and we may simply write

$$E = E_o + \langle F_o | H_p | F_o \rangle \quad (IIIIE24)$$

where, if $E_o \neq -\epsilon$

$$\begin{aligned}
 \langle F_o | H_p | F_o \rangle \Big|_{K_3=0} &= \frac{E_o + \epsilon}{2E_o} (B_{a3}^c \beta_w^* H J + H v_c S) \\
 &= \frac{E_o - \epsilon}{2E_o} (B_{a3}^v \beta_w^* H J - H v_v S) , \quad (IIIIE25a)
 \end{aligned}$$

where we have used Eq. IIIC63 to write

$$b_3 = \beta_w^* H = \frac{|e|\hbar}{m_o c} \frac{(\vec{H} \cdot \overleftrightarrow{m}_w \cdot \vec{H})^{1/2}}{|\overleftrightarrow{m}_w|^{1/2}}, \quad (\text{IIIE25b})$$

where

$$\overleftrightarrow{m}_w = (\overleftrightarrow{\alpha}_w)^{-1}, \quad (\text{IIIE26})$$

and the meaning of $\overleftrightarrow{\alpha}_w$, the Wolff reciprocal mass tensor, was explained at the beginning of this section. These expressions agree with those derived by Baraff. (39)

In the next part of this section, we will show that the transformation properties of B_a^i , B_{33}^i , and v_i are

$$B_a^i = \frac{\vec{H} \cdot \overleftrightarrow{\hat{D}}_i \cdot \vec{H}}{\vec{H} \cdot \overleftrightarrow{m}_w \cdot \vec{H}}, \quad (\text{IIIE27a})$$

$$Hv_i = \frac{\vec{H} \cdot \overleftrightarrow{\hat{F}}_i \cdot \vec{H}}{(\vec{H} \cdot \overleftrightarrow{m}_w \cdot \vec{H})^{1/2}}, \quad (\text{IIIE27b})$$

and

$$B_{33}^i = \frac{\vec{H} \cdot \overleftrightarrow{\hat{T}}_i \cdot \vec{H}}{\vec{H} \cdot \overleftrightarrow{m}_w \cdot \vec{H}}, \quad (\text{IIIE27c})$$

where

$$\overleftrightarrow{T}_i = 2\text{Tr}(\overleftrightarrow{\hat{D}}_i \cdot \overleftrightarrow{\alpha}_w \cdot \overleftrightarrow{m}_w - 4\overleftrightarrow{\hat{D}}_i), \quad (\text{IIIE27d})$$

where the tensors $\overleftrightarrow{\hat{D}}_i$, $\overleftrightarrow{\hat{F}}_i$, and $\overleftrightarrow{\alpha}_w = (\overleftrightarrow{m}_w)^{-1}$ are to be experimentally determined. (39)

It is argued in Section IIC that the experimental fact that the peaks in the magnetorefectivity display no splitting implies that

$$\hat{\vec{D}}_c = -\hat{\vec{D}}_v \equiv \hat{\vec{D}}, \quad (\text{IIIE28a})$$

and

$$\hat{\vec{F}}_c = -\hat{\vec{F}}_v \equiv \hat{\vec{F}}, \quad (\text{IIIE28b})$$

and that therefore similar relations must hold for all quantities related to these tensors. The use of these relationships allows us to greatly simplify the form of Eq. IIIE23, to find

$$\langle F_o | H_p | F_o \rangle = \frac{\epsilon}{E_o} (B_a b_3 J + \frac{1}{2} B_{33} K_3^2) + \hbar v S (1 - \frac{K_3^2 \epsilon}{E_o (E_o + \epsilon)}) \quad (\text{IIIE29})$$

Since the conductivity tensor involves an integral over K_3 , we were interested in exploring the behavior of the bands when $K_3 \neq 0$. This exploration is greatly facilitated by the simple form of Eq. IIIE29. Using degenerate perturbation theory we write F^ℓ , the approximate eigenfunction of $H = H_o + H_p$, as a linear combination of the degenerate solutions of H_o ,

$$F^\ell = C^\ell(1) F_o(S=+1) + C^\ell(-1) F_o(S=-1), \quad (\text{IIIE30})$$

and write the corresponding approximate eigenvalue of H , E_ℓ , as

$$E_\ell = E_o + \Delta E_\ell. \quad (\text{IIIE31})$$

To determine $C^\ell(S)$ and ΔE_ℓ , we solve the secular equation

$$\begin{pmatrix} H_p(1,1)-E_\ell & H_p(1,-1) \\ H_p(-1,1) & H_p(-1,-1)-E_\ell \end{pmatrix} \begin{pmatrix} C^\ell(1) \\ C^\ell(-1) \end{pmatrix} = 0, \quad (\text{IIIE32})$$

where

$$H_p(S,S') \equiv \langle F_o(S) | H_p | F_o(S') \rangle. \quad (\text{IIIE33})$$

Solving for E_ℓ , we obtain

$$E_\ell = E_o + \frac{\epsilon}{E_o} (B_a b_3 J + \frac{1}{2} B_{33} K_3^2) + H_v \ell \sqrt{1 - \frac{K_3^2 \epsilon}{E_o^2}}, \quad (\text{IIIE34})$$

where $\ell = \pm 1$. The expressions for $C^\ell(S)$ can also be found, but are quite complicated, and will not be presented here. They will be discussed in the last part of this section.

Eq. IIIE34 may be even further simplified by defining

$$E'_o \equiv (\epsilon^2 + \epsilon b'_3 J + \epsilon K'^2_3)^{1/2}, \quad (\text{IIIE35})$$

where

$$K'^2_3 \equiv K^2_3 (1 + B_{33}) \quad (\text{IIIE36a})$$

and

$$b'_3 \equiv b_3 (1 + 2B_a). \quad (\text{IIIE36b})$$

Expanding the square root to the same order of approximation as was used in deriving Eq. IIIE34, we find

$$E'_0 = E_0 + \frac{\epsilon}{E_0} (B_a b_3^J + \frac{1}{2} K_3^2 B_{33}) \quad (\text{IIIE37})$$

Discarding the difference between E_0 and E'_0 , K_3 and K'_3 in the small term proportional to v , we may finally write

$$E_\ell = E'_0 + H v \ell \sqrt{1 - \frac{K_3'^2 \epsilon}{E_0'^2}} \quad (\text{IIIE38})$$

when $J \neq 0$. The effect of the second term on the magnetorefectivity spectrum is discussed in Section IIC, and its effect on the magnetorefectivity line-shape, in Section IIIF.

From Eq. IIIE35, we see that the term E'_0 is of precisely the form predicted by the Lax model, and it is clear that when the splitting may not be resolved, and one fits his data to the Lax model for a given orientation of magnetic field, that b_3' is the quantity measured. We still, however, must explore the transformation properties of b_3' to see whether the ellipsoidal model should still apply, since it is not at once clear that b_3' should still transform proportional to $(\vec{H} \cdot \vec{m} \cdot \vec{H})^{1/2}$ due to the complicated transformation properties of B_a . We will explore the transformation properties of b_3' and the quantity $K_3'^2$, which also appears in Eq. IIIE35, in the next part of this section.

First, however, let us explore the effects of the Baraff interaction on the $J = 0$ valence, and the $J = 0$ conduction Landau levels, which we have not yet considered. Although these two Landau levels are not degenerate, they are separated by only the very small energy E_g near $K_3 = 0$. Furthermore, it is found that at high magnetic fields (more than 40 kG), the magnitude of the matrix elements of H_p are of the order of ϵ , and therefore, one would

expect that the $F_0(D=1, J=0)$ and $F_0(D=-1, J=0)$ eigenfunctions of H_0 (where D is the band index) will be strongly mixed by the Baraff interaction near $K_3 = 0$. Fortunately, at these high fields, the other Landau levels are far removed in energy (i.e. $E_0(J \neq 0) \gg \epsilon$), so that one expects to be able to ignore the admixture of any of the $F_0(J \neq 0)$ eigenfunctions of H_0 . One can therefore proceed in almost exactly the same way we did before. We first write $F(d)$, the two approximate $J = 0$ eigenfunctions of the total Baraff Hamiltonian, as the linear combinations

$$F(d) = \sum_{D=-1}^{+1} G^d(D) F_0(D) , \quad (\text{IIIE39})$$

where the quantum number $d=\pm 1$ will label the two solutions. The eigenvalue, E_d , and the corresponding expansion coefficients, $G^d(D)$, are found by solving the secular equation

$$\begin{pmatrix} H(D=1, D'=1) - E_d & H(D=1, D'=-1) \\ H(D=-1, D'=1) & H(D=-1, D'=-1) - E_d \end{pmatrix} \begin{pmatrix} G^d(1) \\ G^d(-1) \end{pmatrix} = 0 , \quad (\text{IIIE40})$$

The diagonal matrix elements in this expression are merely the diagonal matrix elements of the full Baraff Hamiltonian between the eigenfunctions of H_0 , and may be readily found using Eq. IIIE29. When $J = 0$, however, we may greatly simplify this expression by noting that

$$[E_0(J=0)]^2 - \epsilon^2 = \epsilon K_3^2 , \quad (\text{IIIE41})$$

so that we may write

$$H(D,D) = E_0 + \frac{\epsilon}{E_0} [H_0 + \frac{1}{2} B_{33} K_3^2] . \quad (\text{IIIE42})$$

To find the off-diagonal matrix elements, it is convenient to first define

$$E_0 = D\hat{\epsilon} = D \sqrt{\epsilon^2 + \epsilon K_3^2} , \quad (\text{IIIE43})$$

so that $\hat{\epsilon}$ is always a positive quantity. We may then evaluate Eqs. IIID68 and 69 for the $J = 0$ eigenfunctions of H_0 , to obtain

$$F_0(D) = \frac{1}{\sqrt{2\hat{\epsilon}}} \begin{pmatrix} \sqrt{\hat{\epsilon} + D\epsilon} \\ -iD\sqrt{\hat{\epsilon} - D\epsilon} \end{pmatrix} x(n=0, K_3, S=+1) . \quad (\text{IIIE44})$$

The off-diagonal matrix elements can then be written

$$\begin{aligned} \langle F_0(D) | H | F_0(-D) \rangle &= \langle F_0(D) | H_p | F_0(-D) \rangle \\ &= \frac{1}{2\hat{\epsilon}} \begin{pmatrix} \sqrt{\hat{\epsilon} + D\epsilon} \\ -iD\sqrt{\hat{\epsilon} - D\epsilon} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \sqrt{\hat{\epsilon} - D\epsilon} \\ -iD\sqrt{\hat{\epsilon} + D\epsilon} \end{pmatrix} \langle x | \vec{p} \cdot \frac{\vec{B}^c}{2} \cdot \vec{p} + \vec{L}^c \cdot \vec{\sigma} | x \rangle \\ &= \frac{K_3 \sqrt{\epsilon}}{\hat{\epsilon}} \langle x | \vec{p} \cdot \frac{\vec{B}^c}{2} \cdot \vec{p} + \vec{L}^c \cdot \vec{\sigma} | x \rangle \\ &= \frac{K_3 \sqrt{\epsilon}}{\hat{\epsilon}} \left[\frac{1}{2} B_{33} K_3^2 + H_0 \right] , \quad (\text{IIIE45}) \end{aligned}$$

where we have essentially repeated most of the derivation for the $J \neq 0$ matrix elements, making the obvious modifications. The eigenvalues of Eq. IIIE40 may now easily be shown to be

$$E_d = d \sqrt{(\epsilon + H\nu + \frac{1}{2} B_{33} K_3^2)^2 + \epsilon K_3^2} \quad . \quad (\text{IIIE46})$$

It is convenient, at this point, to also write $E_d(J = 0)$ as a function of K_3' in keeping with the conventions of Eq. IIIE38. Since $B_{33}^* \ll 1$, we may write that

$$E_d = \sqrt{(\epsilon + H\nu)^2 + H\nu B_{33} K_3'^2 + \epsilon K_3'^2 + (\frac{1}{2} B_{33} K_3'^2)^2} \quad (\text{IIIE47})$$

to the same order of approximation as was used in deriving Eq. IIIE46. Once again we will defer the discussion of the expressions for $C^d(D)$, the expansion coefficients, until the last part of this section.

Finally, let us compare Eq. IIIE47 with the expressions derived by Baraff. He only considered the $k_H = 0$ case and found

$$E_{\text{conduction}} = \epsilon + H\nu , \quad (\text{IIIE48a})$$

and

$$E_{\text{valence}} = -\epsilon - H\nu , \quad (\text{IIIE48b})$$

in agreement with the expressions above. We have therefore completed our justification of the equations which appear in Section IIC of this thesis.

* This estimate is justified at the end of the second part of this section.

TRANSFORMATION PROPERTIES

We will now consider the transformation properties of the quantities in the previously derived equations. The central problem is to find R_{ij} , the matrix defined by Eq. IIID50, which relates the field independent quantities such as $\hat{B}_{ij}$ and $\vec{X}(j)$, (See Eqs. IIIE5 and D8) to the field dependent ones such as B_{ij} and $\vec{W}(j)$ (See Eqs. IIIE8 and D50). It turns out that we require only the third row of this matrix, R_{3j} .

Let us first relate our choice of the vectors $\vec{W}(j)$ to the direction of the magnetic field in a more explicit way than we have done previously. The simplest way to choose these vectors so that $b_1 = b_2 = 0$ is to simply require $\vec{W}(3)$ to be parallel to $\vec{H}$, so we may write

$$\vec{H} = a\vec{H}\vec{W}(3), \quad (\text{IIIE49})$$

where a is some constant which we must find. We may make b_3 positive merely by choosing the sign of $\vec{W}(2)$. To completely evaluate $\vec{W}(3)$ as a function of $\vec{H}$, we use Eqs. IIIC34 and 63 to write

$$\begin{aligned} b_3 &= \frac{|e|\hbar}{m_o c} \frac{(\vec{H} \cdot \vec{m}_w \cdot \vec{H})^{1/2}}{|\vec{m}_w|^{1/2}} = \vec{H} \cdot \vec{W}(1) \times \vec{W}(2) \frac{e\hbar}{m_o c} \\ &= a\vec{H}\vec{W}(3) \cdot \vec{W}(1) \times \vec{W}(2) \frac{e\hbar}{m_o c}, \end{aligned} \quad (\text{IIIE50})$$

where $\vec{m}_w$ is the reciprocal of $\vec{\alpha}_w$ which was defined in Eq. IIIE2b. It can be shown that

$$-\vec{W}(1) \times \vec{W}(2) \cdot \vec{W}(3) = |\vec{\alpha}_w|^{1/2} = \frac{1}{|\vec{m}_w|^{1/2}} \quad (\text{IIIE51})$$

so using Eqs. III E50 and 51, we may write

$$\frac{\vec{H}}{aH} = \frac{\vec{H}}{(\vec{H} \cdot \vec{m}_w \cdot \vec{H})^{1/2}} = \vec{W}(3) , \quad (\text{III E52})$$

It is also convenient to define three real space vectors, $\vec{Q}(j)$, such that

$$\vec{Q}(j) \cdot \vec{X}(j') = \delta_{jj'} , \quad (\text{III E53a})$$

or equivalently

$$\sum_j Q_\alpha(j) X_\beta(j) = \delta_{\alpha\beta} . \quad (\text{III E53b})$$

In terms of these field independent vectors we may finally find R_{3j} by using Eqs. III E52 and D50 to write

$$\vec{Q}(j) \cdot \vec{W}(3) = \frac{\vec{H} \cdot \vec{Q}(j)}{(\vec{H} \cdot \vec{m}_w \cdot \vec{H})^{1/2}} = \vec{Q}(j) \cdot \sum_j R_{3j} \vec{X}(j') = R_{3j} . \quad (\text{III E54})$$

Using this equation and Eq. III E8b, we may find the transformation properties of L_3 ,

$$L_3 = \sum_j R_{3j} \mathcal{L}_j = \frac{\vec{H} \cdot \vec{T}^a \cdot \vec{H}}{(\vec{H} \cdot \vec{m}_w \cdot \vec{H})^{1/2}} , \quad (\text{III E55})$$

where using Eq. III D6 to define $\vec{\mathcal{L}}$,

$$T_{\gamma\beta}^a = (\text{Re}\{Y_\gamma\} Q_\beta(1) - \text{Im}\{Y_\gamma\} Q_\beta(2) + M_\gamma Q_\beta(3)) . \quad (\text{III E56})$$

We see L_3 depends only on the symmetric part of $\vec{T}^a$. Furthermore, it must be invariant under a two-fold rotation around the binary axis, due to the symmetry properties of the L point in the Brillouin zone. Therefore, for the

principal ellipsoid, we may write $\overset{\leftrightarrow}{T}^a$ as a function of four independent parameters,

$$\overset{\leftrightarrow}{T}^a = \begin{pmatrix} T_1^a & 0 & 0 \\ 0 & T_2^a & T_4^a \\ 0 & T_4^a & T_3^a \end{pmatrix} . \quad (\text{IIIE57})$$

We may also find B_{33} in a similar manner by substituting in Eq. IIIE8a

$$B_{33} = \sum_{j,l} R_{3j} \hat{B}_{jl} R_{3l} = \frac{\vec{H} \cdot \overset{\leftrightarrow}{T}^b \cdot \vec{H}}{\vec{H} \cdot \underset{w}{m} \cdot \vec{H}} , \quad (\text{IIIE58})$$

where the new tensor, $\overset{\leftrightarrow}{T}^b$, is defined as

$$\overset{\leftrightarrow}{T}^b_{\beta\gamma} = \sum_{j,l} Q_{\beta}(j) \hat{B}_{jl} Q_{\gamma}(l) , \quad (\text{IIIE59})$$

and is also of the form of Eq. IIIE57.

We now must find B_a . Using the definition of Eq. E13a, we may write

$$B_a = \frac{1}{4} (\text{Tr}\{\overset{\leftrightarrow}{B}\} - B_{33}) . \quad (\text{IIIE60})$$

To evaluate $\text{Tr}\{\overset{\leftrightarrow}{B}\}$ we calculate

$$\begin{aligned} \text{Tr}\{\overset{\leftrightarrow}{\alpha}_w \cdot \overset{\leftrightarrow}{T}^b\} &= \sum_{\gamma, j, j', l} X_{\gamma}(j) \vec{X}(j) \cdot \vec{Q}(j') \hat{B}'_{jl} Q_{\gamma}(l) \\ &= \text{Tr}\{\overset{\leftrightarrow}{\hat{B}}\} = \text{Tr}\{\overset{\leftrightarrow}{B}\} , \end{aligned} \quad (\text{IIIE61})$$

where we have used Eq. IIIE53, and the fact that $\text{Tr}\{\overset{\leftrightarrow}{R} \cdot \overset{\leftrightarrow}{B} \cdot \overset{\leftrightarrow}{R}^T\}$ is an invariant of the transformation $\overset{\leftrightarrow}{R}$.

Therefore for B_a , we finally find

$$B_a = \frac{\vec{H} \cdot \vec{\hat{D}} \cdot \vec{H}}{\vec{H} \cdot \vec{m}_w \cdot \vec{H}} \quad , \quad (\text{IIIE62})$$

where

$$\vec{\hat{D}} \equiv \frac{1}{4} (\text{Tr} \{ \vec{\alpha}_w \cdot \vec{T}^b \} \vec{m}_w - T^b) \quad , \quad (\text{IIIE63})$$

Similar relations also exist between B_a^v , B_a^c , $\vec{\hat{D}}^v$ and $\vec{\hat{D}}^c$. Finally we may evaluate v , defined by Eq. IIIE22, as

$$Hv = \frac{\vec{H} \cdot \vec{\hat{F}} \cdot \vec{H}}{(\vec{H} \cdot \vec{m}_w \cdot \vec{H})^{1/2}} \quad , \quad (\text{IIIE64})$$

where we have used Eq. IIIE25b to define

$$\vec{\hat{F}} \equiv \vec{T}^a + \vec{\hat{D}} \frac{|e| \hbar}{m_o c |\vec{m}_w|^{1/2}} \quad , \quad (\text{IIIE65})$$

Once again, similar relations also exist between v_c , v_v , $\vec{\hat{F}}_c$ and $\vec{\hat{F}}_v$.

Let us now explore the transformation properties of b'_3 . If we define

$$\vec{m}^* \equiv \frac{(\vec{m}_w + 4\vec{\hat{D}}) |\vec{m}_w|^{1/2}}{|\vec{m}_w + 4\vec{\hat{D}}|^{1/2}} \quad (\text{IIIE66a})$$

and

$$\beta^*_H \equiv \frac{\hbar |e| (\vec{H} \cdot \vec{m}^* \cdot \vec{H})^{1/2}}{m_o c |\vec{m}^*|^{1/2}} = \frac{\hbar |e| (\vec{H} \cdot [\vec{m}_w + 4\vec{\hat{D}}] \cdot \vec{H})^{1/2}}{m_o c |\vec{m}_w|^{1/2}} \quad , \quad (\text{IIIE66b})$$

we may expand the square root to lowest order in $\hat{D}$ and find

$$\begin{aligned}\beta^* H &= \frac{\hbar |e| (\vec{H} \cdot \vec{m}_w \cdot \vec{H})^{1/2}}{m_0 c |\vec{m}_w|^{1/2}} \left(1 + 2 \frac{\vec{H} \cdot \hat{D} \cdot \vec{H}}{\vec{H} \cdot \vec{m}_w \cdot \vec{H}} \right) \\ &= b_3 (1 + 2B_a) = b'_3\end{aligned}\quad (\text{IIIE67})$$

according to the definition of Eq. E36b. Therefore b'_3 can be written as $\beta^* H$, where β^* transforms in the same way as in the Lax model, and therefore the effective mass m^* involved in Eq. IIIE66b is the one which is usually determined by fitting experimental data to the Lax model. It should be noted that as a result of the experimental fact that the peaks in the magneto-reflectivity are not split (See Eqs. IIIE28a and b and the pertinent argument in Section IIC), these conclusions concerning the Lax model are true even though the full Baraff Hamiltonian has been solved to first order in perturbation theory.

To find $\hat{F}$ we would measure the orientation dependence of v and fit it to Eq. IIIE64, ignoring the small difference between $\vec{m}^*$ and $\vec{m}_w$. The tensor $\hat{F}$ also has only four independent parameters, and the form given by Eq. IIIE57.

For completeness, we will also evaluate the transformation properties of K_3^2 and $K_3'^2$. It is clear, however, that these quantities are both proportional to the square of k_H , the component of the crystalline momentum parallel to the magnetic field, with a proportionality constant dependent on magnetic field orientation but not magnetic field magnitude, so that these transformation properties essentially determine nothing more than the field orientation dependence of the density of states per unit K_3 or K_3' .

We will first consider K_3^2 . From the definition of K_3 in Eq. IIID17b, we may write

$$K_3^2 = \frac{\hbar^2}{m_0} \sum_{jj'} R_{3j} \vec{X}(j) \cdot \vec{k} R_{3j'} \vec{X}(j') \cdot \vec{k} = \frac{\hbar^2}{m_0} \frac{(\vec{H} \cdot \vec{k})^2}{(\vec{H} \cdot \vec{m}_w \cdot \vec{H})}, \quad (\text{IIIE68})$$

where we have substituted Eq. IIIE54 for R_{3j} and used Eq. III53 to do the sum. Therefore, for K_3^2 we get the expected result

$$K_3^2 = \frac{\hbar^2}{m_0 m_{Hw}} k_H^2, \quad (\text{IIIE69})$$

where

$$m_{Hw} = \frac{\vec{H} \cdot \vec{m}_w \cdot \vec{H}}{H^2}, \quad (\text{IIIE70})$$

and k_H is the crystalline momentum parallel to the magnetic field. For $K_3'^2$ we may define the analogous quantity, m_H , by the relation

$$\frac{\hbar^2}{m_0 m_H} k_H^2 \equiv K_3'^2 = K_3^2 (1 + B_{33}), \quad (\text{IIIE71})$$

where we have used Eq. IIIE36a to define K_3' . Furthermore, we can prove that m_H may be determined by an equation analogous to Eq. IIIE70; namely

$$m_H = \frac{\vec{H} \cdot \vec{m}^* \cdot \vec{H}}{H^2}. \quad (\text{IIIE72})$$

To do this, we first substitute Eq. IIIE58 for B_{33} in Eq. IIIE71 to obtain

$$\frac{1}{m_H} = \frac{1}{m_{Hw}} \left(1 + \frac{\vec{H} \cdot \vec{T} \cdot \vec{H}}{\vec{H} \cdot \vec{m}_w \cdot \vec{H}} \right), \quad (\text{IIIE73})$$

which shows, that to first order

$$m_H = \vec{H} \cdot (\vec{m}_W - \vec{T}^b) \cdot \vec{H} / H^2 \quad . \quad (\text{IIIE74})$$

Next, it is convenient to find $\vec{T}^b$ in terms of the tensors $\vec{m}_W$ and $\hat{D}$ which appear in our definition of $\vec{m}^{**}$ in Eq. IIIE66a. To do this, we may use Eq. IIIE63, and obtain the result

$$\vec{T}^b = 2\text{Tr}\{\hat{D} \cdot \vec{\alpha}_W\} \vec{m}_W - 4\hat{D} \quad . \quad (\text{IIIE75})$$

Working in the coordinate system in which the tensors $\vec{m}_W$ and $\vec{\alpha}_W$ are diagonal, we now may show

$$\vec{m}_W - \vec{T}^b = \vec{m}_W (1 - 2 \sum_j \alpha_{jj}^W \hat{D}_{jj}) + 4\hat{D} \quad . \quad (\text{IIIE76})$$

Furthermore, upon expanding Eq. IIIE66a to the first order in the small quantities $\hat{D}_{ij}$, we find that in this coordinate system $\vec{m}^{**}$ is also equal to the right side of Eq. IIIE76, completing our proof of Eq. IIIE72.

Let us now combine Eqs. IIIE38 and 47 with the transformation relations we have developed to write equations for the Landau level energies, including the Baraff terms, which involve only field independent parameters. If we drop the prime from E'_0 , and define j , the Landau level total angular momentum quantum number by

$$j \equiv J/2 \quad , \quad (\text{IIIE77})$$

we may write Eq. IIIE38, where $j \neq 0$, as

$$E_\ell = E_0 + H \nu \ell \sqrt{1 - \frac{k_H^2 E_0^2}{2m_0 m_H E_0^2}} \quad , \quad (\text{IIIE78})$$

where

$$E_0 = \sqrt{\frac{E_g^2}{4} + E_g (\beta^*_{Hj} + \frac{\hbar^2}{2m_0 m_H} k_H^2)} , \quad (\text{IIIE79a})$$

$$\beta^*_{Hj} = \frac{\hbar |e|}{m_0 c} \frac{(\vec{H} \cdot \vec{m}^* \cdot \vec{H})^{1/2}}{|\vec{m}^*|^{1/2}} , \quad (\text{IIIE79b})$$

$$m_H = \frac{\vec{H} \cdot \vec{m}^* \cdot \vec{H}}{H^2} , \quad (\text{IIIE79c})$$

and

$$Hv = \frac{\vec{H} \cdot \vec{F} \cdot \vec{H}}{(\vec{H} \cdot \vec{m}^* \cdot \vec{H})^{1/2}} . \quad (\text{IIIE79d})$$

The tensors, $\vec{m}^*$ and $\vec{F}$ may be easily determined by experiment.

Proceeding in a similar manner for the $j = 0$ Landau levels, using Eq. IIIE47, one finds

$$E_d = d \sqrt{\left(\frac{E_g}{2} + Hv\right)^2 + \frac{\hbar^2}{2m_0 m_H} k_H^2 (E_g + 2HvB_{33} + \frac{\hbar^2}{2m_0 m_H} [B_{33}k_H]^2)} , \quad (\text{IIIE80})$$

where $d = \pm 1$ for conduction and valence bands, respectively;

$$B_{33} = \frac{\vec{H} \cdot \vec{T}^b \cdot \vec{H}}{\vec{H} \cdot \vec{m}^* \cdot \vec{H}} , \quad (\text{IIIE81})$$

and where the other parameters were defined in Eq. IIIE79.

The explicit appearance here of $\vec{T}^b$ is quite troublesome, since this tensor would be very difficult to measure experimentally. We will therefore relate it to β , since we have some idea as to the magnitude of this tensor.

This can be done by first calculating $\overleftrightarrow{T}^b$ by utilizing Eqs. III E5 and 59 and the easily proven relation

$$\sum_j Q_u(j) Q_v(j) = m_{uv}^w \quad (\text{III E82})$$

to obtain

$$\overleftrightarrow{T}^b = \overleftrightarrow{m}_w \cdot \overleftrightarrow{\beta} \cdot \overleftrightarrow{m}_w \quad (\text{III E83})$$

Next, we note that $\overleftrightarrow{m}_w$ is a highly anisotropic tensor, so that B_{33} is approximately given by the relation

$$B_{33} = (\overrightarrow{B} \cdot \overleftrightarrow{m}_w \cdot \overrightarrow{B}) (\overrightarrow{B} \cdot \overleftrightarrow{\beta} \cdot \overrightarrow{B}) , \quad (\text{III E84})$$

provided that the tensor $\overleftrightarrow{\beta}$ is much less anisotropic than $\overleftrightarrow{m}_w$, and that the magnetic field is more than a degree or two away from being perpendicular to $\overrightarrow{B}$, the unit vector parallel to the long axis of the electron pockets. Ignoring the small difference between $\overleftrightarrow{m}_w$ and $\overleftrightarrow{m}^*$ in estimating the small quantity B_{33} , (See Table II for the measured values of $\overleftrightarrow{m}^*$) and using the estimate $\overrightarrow{B} \cdot \overleftrightarrow{\beta} \cdot \overrightarrow{B} \leq 1/2$ given at the beginning of this section, we find that B_{33} is on the order of .1 or less.

In Figure 14 we have plotted solid lines for the Landau level energy vs. k_H for a fixed value of magnetic field, using Eqs. III E78 and 80. At a high value of k_H , of course, the first order degenerate perturbation theory used in deriving these equations will no longer be accurate, but since it is known that the deviations from the Lax model at the Fermi surface are rather small, these expressions should be adequate to values of k_H on the order of k_F . The parameters used in generating Figure 14 were taken from Table II, and B_{33} was

set equal to .1. The magnetic field is along the binary axis, and the curves are for the bands associated with the light electron pockets. The energies predicted by the Lax model for the same m^* are also shown as dashed lines in Figure 14 for comparison.

BARAFF VELOCITY MATRIX ELEMENTS

We would now like to calculate the velocity matrix elements between the eigenfunctions corresponding to the Baraff Landau levels of Figure 14. One would expect, as a matter of fact, that these velocity matrix elements would differ greatly from the velocity matrix elements between the eigenfunctions corresponding to the Lax Landau levels, calculated from the Wolff Hamiltonian in Section IIID. We would expect this because we found, in the first part of Section IIIE, that the eigenfunctions, $F_0(D,S)$, of the Wolff Hamiltonian, differ in zeroth order from $F(D,S)$, the corresponding eigenfunctions of the Baraff Hamiltonian. In this part of this section we will therefore go about calculating the Baraff velocity matrix elements. We will find that for the interband transition, the Baraff and Wolff velocity matrix elements are actually quite similar, so that it is worth while carrying out the calculation set up in Section IIID in order to get the theoretical estimate of the magnetoreflectivity lineshape presented in Section IIIF.

Let us first consider those transitions which involve the $j = 0$ Landau level. To simplify the problem, we note that we need consider only the $\chi(+)$ component of the effective mass velocity operator, as discussed in Section IIID. Since this operator couples states such that $j_2 = j_1 + 1$, we find that $j_1 = 0$ and $j_2 = 1$ for the transitions under discussion. To calculate the Baraff velocity matrix elements for these transitions, we note that since we

may write the Baraff eigenfunctions as linear combinations of the Wolff eigenfunctions, (See Eqs. IIIE30 and 39) we may write the Baraff velocity matrix elements as linear combinations of the Wolff velocity matrix elements;

$$\langle F(j_1, S_1, D_1) | \chi(+) | F(j_2, S_2, D_2) \rangle = \sum_{d, \ell} G^D(d) \langle F_0(j_1, S_1, d) | \chi(+) | F_0(j_2, \ell, D_2) \rangle C^S(\ell). \quad (\text{IIIE85})$$

It should be noted that since $j_1 = 0$, S_1 must equal +1, as was discussed in Section IIC. The expansion coefficients, $G^D(d)$ and $C^S(\ell)$, may now be obtained by solving Eqs. IIIE32 and 40 to obtain the relations

$$C^S(\ell) = \ell \sqrt{\frac{1}{2} + \frac{S\ell}{2} \frac{(E_0 + \epsilon) E_0 - \epsilon K_3^2}{(E_0 + \epsilon) \sqrt{E_0^2 - \epsilon K_3^2}}} \quad (\text{IIIE86a})$$

and

$$G^D(d) = d \sqrt{\frac{1}{2} + \frac{dD}{2} \frac{\hat{\epsilon}^2 + \epsilon(H\nu + \frac{1}{2} B_{33} K_3^2)}{\hat{\epsilon} \sqrt{(\epsilon + H\nu + \frac{1}{2} B_{33} K_3^2)^2 + \epsilon K_2^2}}} \quad (\text{IIIE86b})$$

where

$$\hat{\epsilon} = |E_0(j=0)| = + \sqrt{\epsilon^2 + \epsilon K_3^2}. \quad (\text{IIIE86c})$$

Using the expressions for the Wolff velocity matrix elements derived in Section IIID, it is now quite simple to calculate the Baraff velocity matrix elements.

The results of such a calculation are presented in Figure 21a. Here we plot $\frac{m_0}{\epsilon} |\langle \chi(+) \rangle|^2$, the normalized velocity matrix element squared, as a function

of k_H for both the Baraff (solid lines) and the Wolff (dashed lines) relations. In particular, we have presented graphs for all of the inter-Landau level transitions, allowed near $k_H = 0$, which involve the $j = 0$ Landau levels. As in Figure 14, we have assumed a field of 50 kG along the binary axis, and that the states under consideration are associated with the light electron ellipsoids.

We will first discuss the two anomalous interband transitions, which involve the ($j = 0$, valence) Landau level. These transitions make the main contribution to the $n = 0$ interband oscillation. They are called anomalous because at $k_H = 0$, the spin conserving transition is zero and the spin flipping transition is large, in contrast to normal transitions where at $k_H = 0$ the spin conserving transition is large and the spin flipping transition is zero. Only transitions involving the ($j = 0$, valence) Landau level have this anomalous characteristic.

The most important thing to note about the anomalous interband transitions is that for the spin flipping one, the Baraff and Wolff velocity matrix elements are quite similar, even though the Wolff and Baraff eigenfunctions differ in zeroth order when $k_H \neq 0$. We therefore conclude, as a result of this similarity, that for the spin flipping anomalous interband transition, the contribution to the conductivity calculated from the simpler Wolff model should be a reasonable approximation to the conductivity calculated using the more accurate Baraff model.

For the anomalous spin conserving interband transition, the discrepancies between the Wolff and Baraff velocity matrix elements are much larger. A numerical calculation (See Section IIIF) shows, however, that this transition contributes very little to the $n = 0$ oscillation lineshape, because for this

transition, the velocity matrix element is very small for small k_H , where there is a peak in the joint density of states. It therefore seems reasonable to assume that the $n = 0$ oscillation lineshape is determined mainly by the anomalous spin flipping interband transition, and therefore seems reasonable to expect that the theory of Section IIID will give reasonable agreement with experiment for this resonance. The agreement between theory and experiment is discussed in detail in Section IIIF, where this, in fact, is found to be the case.

At the bottom of Figure 21a, we present graphs for the normal intraband transitions which involve the ($j = 0$, conduction) Landau level. These transitions are responsible for the cyclotron resonance line. The most important thing to note here is that there is a large difference between the Wolff and Baraff velocity matrix elements for both the spin flipping, and spin conserving intraband transitions. We therefore would conclude that the calculation of Section IIID, based on the Wolff model, should give poor agreement with the experimentally observed cyclotron resonance line. This is also found to be the case. Furthermore, it can be argued that the use of the more accurate Baraff formulas should greatly improve the agreement. This matter will also be discussed in some detail in Section IIIF.

In Figure 21b, we present graphs for the velocity matrix elements associated with the normal interband ($j_1 = 1, j_2 = 2$) transitions. These graphs are representative of all of the remaining interband transitions, which do not involve the $j = 0$ Landau levels. Since there are eight individual interband transitions associated with the ($j_1 = 1, j_2 = 2$) interband transitions (See Figure 12), we do not, in this case, present individual graphs for each one as we did for the $j = 0$ velocity matrix elements in Figure 21a.

Instead, we have first divided the eight transitions into three groups, according to the way which they are shifted by the Baraff interaction, and have then calculated the total effective velocity matrix element for each group. For example, we have found that the four spin conserving interband transitions remain degenerate and unshifted in resonance energy when the Baraff interaction is included in the calculation, and have therefore defined $|\langle B | \chi(+) | B \rangle|_{SC}^2$, the total effective velocity matrix element squared for the spin conserving transitions between the Baraff eigenfunctions, by the equation

$$|\langle B | \chi(+) | B \rangle|_{SC}^2 = \sum_{S,D} |\langle F(D,S) | \chi(+) | F(-D,S) \rangle|^2 \quad (\text{IIIE87a})$$

and plotted the normalized result, $\frac{m_o}{\epsilon} |\langle B | \chi(+) | B \rangle|_{SC}^2$, at the solid line in the topmost graph of Figure 21b. For comparison, we have also plotted the corresponding quantity for the Wolff model,

$$\frac{m_o}{\epsilon} |\langle w | \chi(+) | w \rangle|_{SC}^2 = \frac{m_o}{\epsilon} \sum_{S,D} |\langle F_o(D,S) | \chi(+) | F_o(-D,S) \rangle|^2 \quad (\text{IIIE87b})$$

as the dashed line in this graph.

In a similar manner, we have found that two of the spin flipping transitions remain degenerate, but have their resonance energies shifted upwards by the Baraff interaction, while the remaining two spin flipping transitions have their resonance energies shifted downwards by exactly the same amount. Using definitions analogous to those of Eqs. IIIE87a and b, we have drawn the curves for the shifted up, and shifted down spin flipping transitions in the lower part of Figure 21b. It should be noted that once again, the differences

between the Wolff and Baraff velocity matrix elements are relatively small, so that the contribution to the conductivity calculated from the simpler Wolff model should be a reasonable approximation to the conductivity calculated using the more accurate Baraff model.

So far, we have restricted our discussion to the zeroth order changes in the velocity matrix elements produced by the Baraff interaction. There are, of course, also first order effects. One such effect would be a slight further modification of the velocity matrix elements already discussed. This first order modification should be a good deal smaller than the zeroth order modifications already discussed, and therefore should not greatly modify the essential features of the curves of Figure 21. In addition to this first order effect, there would also be a first order breakdown in the selection rules for the Lax model. In other words, we would expect to find non-zero velocity matrix elements for transitions normally forbidden by the Lax model, with magnitudes proportional to the strength of the Baraff interaction. The conductivity, however, involves the velocity matrix elements squared, so that such a breakdown in the selection rules would produce a contribution to the conductivity which would only be of second order in the perturbation. One would therefore expect that such effects should be small, and as a matter of fact, we have never definitely observed any peaks in the reflectivity associated with such a breakdown in the selection rules. We therefore conclude that the first order effects can be completely ignored.

SECTION IIIF

THEORETICAL RESULTS

In this section, we will compare the results of the lineshape calculation set up in Section IIID with the experimental data. In order to obtain numerical results, however, we must first choose a large number of parameters. Most of these parameters are fixed by information available from the magnetoreflexion spectrum and from DHVA, CR and zero field reflectivity experiments, and we will discuss the determination of these parameters in the first part of this section. In the second part we will discuss the fit that can be obtained between the experimental and theoretical lineshapes by varying the only remaining undetermined parameters, the relaxation times. We will find that the fit is reasonably good for the interband oscillations, and present detailed conductivity curves for the interband transitions in the third part of this section. We will also find, however, that there are some striking discrepancies between the theoretical and experimental cyclotron resonance lineshapes. We will discuss these discrepancies in the last part of this section.

CHOOSING THE FIXED PARAMETERS

In this part of the section we will discuss the choice of those parameter values which are fixed by information available from the magnetoreflexivity spectrum, and from DHVA,⁽⁴⁰⁾ CR,⁽⁶⁴⁾ and zero field reflectivity⁽⁷⁰⁾ measurements. These parameters are: E_g , the energy gap; $\vec{m}^*$, the effective mass tensor for the electrons at the bottom of the band; $\vec{m}_h^*$, the effective mass tensor for the holes; g^* , the effective g factor for the holes; $\hat{\epsilon}_{0.L.}$, the

energy band overlap; and finally ϵ , the core dielectric constant corresponding to a given value of ϵ_u , the high energy limit of applicability of the two-band model (See Table II).

First of all, our magnetorefectivity experiments have determined that $E_g = .011 \pm .001$ eV. We have also measured β^* for several orientations of the magnetic field. We still, however, do not have enough information to completely determine $\vec{m}^*$. In particular, we have not measured the dependence of β^* on the angle of the magnetic field in the bisectrix-trigonal plane, and therefore do not know the tilt angle, θ_t , between the bisectrix and the $\vec{B}$ axis, where we have defined the $\vec{B}$ axis as being parallel to the long axis of the principal ellipsoid. Also, we have not observed any oscillations where β^* was small enough to be significantly dependent on the value of $\vec{B} \cdot \vec{m}^* \cdot \vec{B}$, the large component of the effective mass tensor along the $\vec{B}$ axis.

To obtain this information, we have used the recent accurate DHVA measurements of Bhargava,⁽⁴⁰⁾ who found that the Fermi surface is almost exactly ellipsoidal, with a tilt angle of $\theta_t = 6.5^\circ$. To find $\vec{B} \cdot \vec{m}^* \cdot \vec{B}$ we use the ratio between the large extremal area measured with $\vec{H}$ parallel to the binary axis, and the small extremal area, measured with $\vec{H}$ parallel to the $\vec{B}$ axis. Bhargava found that this ratio is 16.4. We now have enough information to completely determine the $\vec{m}^*$ tensor, which is displayed in Table II.

Most of the parameters associated with the holes were taken from the data of Smith, Baraff, and Rowell⁽³⁷⁾ (SBR).^{*} In particular, we have used their

* We did not use their electron parameters because of the limited number of electron oscillations displayed in their high field DHS data.

values for $\overleftrightarrow{m}_h^*$ and $\overleftrightarrow{m}_s^*$, where $\overleftrightarrow{m}_s^*$, the spin effective mass tensor for the holes, is proportional to the $\overleftrightarrow{G}$ tensor of Section IIIC, and is related to g^* by the equation

$$H g^* = 2 \frac{(\vec{H} \cdot \overleftrightarrow{m}_s^* \cdot \vec{H})^{1/2}}{|\overleftrightarrow{m}_s^*|^{1/2}} \quad . \quad (\text{IIIF1})$$

We have also chosen the overlap energy $\hat{\epsilon}_{0.L.} = .044$ eV, so as to obtain a zero field carrier concentration of 2.75×10^{17} holes/cc, in agreement with the value measured by Smith, Baraff, and Rowell.

We must choose $\hat{\epsilon}_u$, the energy beyond which our band model is no longer applicable for the electrons (See Section IIID.) Since we can observe oscillations with well defined lineshapes up to about $\hbar\omega = .35$ eV, we will make $\hat{\epsilon}_u = .2$ eV. (It was found that varying $\hat{\epsilon}_u$ from .2 to .7 eV has essentially no effect on the theoretical reflectivities as long as the corresponding $\overleftrightarrow{\epsilon}$ tensor was used.) To find $\overleftrightarrow{\epsilon}$ corresponding to this value of $\hat{\epsilon}_u$, we fit our theoretical curves to the zero field transmission experiments carried out by Boyle and Brailsford⁽⁷⁰⁾ near the plasma frequency. The good agreement between theory and experiment displayed in Figure 16 was obtained with the parameters $\epsilon_{\parallel \text{Trig}} = 29$ and $\epsilon_{\perp \text{Trig}} = 72$.

THE THEORETICAL AND EXPERIMENTAL LINESHAPES

In this part of this section, we will discuss the fitting of the theoretical lineshapes to the ones determined by experiment. We will find that we can obtain a reasonable fit to all of the interband transition lineshapes, including the peculiar $n = 0$ transition lineshape. The fit to the

cyclotron resonance lineshape, however, is much worse.

Before we can compare the theoretical and experimental results, however, we must first take into account the fact that the output of our monochromators is partially polarized (See Section IIA). The simplest way to do this is to calculate the magnetorefectivity assuming a suitable value for the polarization ratio. In particular, for the binary sample orientation, we will assume that 30% of the incident beam is polarized with the electric field vector of the light parallel to the bisectrix axis.* For the trigonal data, of course, by symmetry the polarization of the light makes no difference. Although the polarization effects are large for the bisectrix sample orientation, we have not done any theoretical calculations for this case for reasons discussed in Appendix F.

We are now ready to attempt to fit the theoretical curves to the experimental ones by adjusting the hole and electron relaxation times, which are the only parameters we have left to vary. We began by getting an overall feel for the problem by calculating the reflectivity for a wide range of fields and photon energies. First of all, we found that the results were relatively insensitive to the choice of the hole relaxation time, so for this parameter

* Unfortunately, it is experimentally difficult to either measure accurately the polarization ratio, or to do the experiment with polarized light with a signal to noise ratio adequate for a detailed lineshape analysis. From the experimental work we have done, however, the value of 30% seems to be a quite reasonable one. Furthermore, it was found that, although the theoretical lineshape is only weakly dependent upon the polarization ratio, so that the value we assign to this quantity is not crucial, it does seem to be true that we obtain the best agreement between theory and experiment for this value of the polarization ratio.

we just used the value $\frac{\hbar}{\tau_H} = .0008 \text{ eV}$, which was determined from the zero field analysis (See Figure 16). It was found, furthermore, that the agreement between theory and experiment could be improved by allowing the relaxation time associated with the spin-flipping transitions, which we will call τ_F , to differ from the relaxation time associated with the corresponding spin conserving transitions, which we will call τ_c . Since these two relaxation times correspond to two physically distinct processes, this inequality is not unreasonable. We do not, however, make any distinction between relaxation times for intra- and interband transitions, since, even at low magnetic fields the two bands are strongly mixed, with the magnetic energy much greater than the energy band gap.

As a result of these preliminary calculations, it soon became apparent that the features in the reflectivity most sensitive to our choice of parameters were the lineshapes of the $n = 0$ interband, and the cyclotron resonance transitions. In attempting to obtain a detailed fit, we therefore concentrated on achieving agreement between the theory, and the experimental lineshape shown in Figure 5. There are several reasons for the choice of this particular piece of data. First of all, the frequency chosen is a convenient one, at which the features of interest occur at high fields where they can be clearly seen. Also, the energy resolution is quite good, due to the use of the high resolution grating monochromator. Considering the small amount of signal energy available, due to the high resolution used, the signal to noise ratio is also satisfactory.

The sort of fit that can be obtained using the Lax model is shown in Figure 17, where we have set $\frac{\hbar}{\tau_c} = .002 \text{ eV}$ and $\frac{\hbar}{\tau_F} = .001 \text{ eV}$. As can be

seen, there is reasonable agreement between the theoretical and experimental lineshapes for the $n = 0$ interband transition oscillation. (See Figure 5 for the experimental data.) In particular, we find that, in agreement with the experimental data, the high-field side of the $n = 0$ oscillation is the steep side, in contrast with the $n \neq 0$ oscillations, where the low field side is the steep side (See Figure 4). For the $n = 0$ interband transition, therefore, our calculation represents an improvement on the calculation of Dresselhaus and Dresselhaus, who assumed simple parabolic bands.⁽²⁸⁾ Their calculation, though it does give the proper lineshape for the $n \neq 0$ oscillations, does not give the proper lineshape for the $n = 0$ oscillation.

Although we have obtained a reasonable fit for the $n = 0$ interband transition oscillation, there is very poor agreement between the theoretical and observed lineshapes for the cyclotron resonance oscillation. In particular, the dip in the reflectivity just below the cyclotron resonance critical field is predicted to be much too large, and furthermore, the knee in the reflectivity curve just above the cyclotron resonance critical field is predicted to be much less sharp than the one actually observed. It should be noted, however, that poor as the agreement between theory and experiment may be for this oscillation, our calculation still represents an improvement with the respect to the results which would be obtained with a simple parabolic band model. More specifically, at photon energies this far above the plasma frequency ($\hbar\omega_p \approx .02$ eV) such a simple model would predict that the cyclotron resonance transition should produce a sharp peak in the reflectivity rather than the shoulder which is observed.

We will discuss the cyclotron resonance oscillation in some detail in the last part of this section, where we will discuss the discrepancies between the

theoretical and experimental lineshapes. At this point, however, let us return to a discussion of the $n = 0$ interband transition oscillation, where the discrepancies are relatively small. The largest disagreement, in this case, lies in the fact that the amplitude of the theoretical oscillation is about twice the amplitude of the $n = 0$ oscillation which is experimentally observed. It is possible to fit the theory to the amplitude of the observed oscillation rather than its lineshape, but one obtains a much poorer overall fit in that case, not only with respect to the data of Figure 5, but also with respect to the data obtained at other fields and photon energies. Since we have found that the amplitude of the oscillations is not particularly reproducible experimentally, we have not made any great attempts to reduce the discrepancy in the amplitudes.

Let us now consider the values we have chosen for τ_F and τ_c . It can be seen that they are much shorter than the value obtained for the electronic relaxation time from the zero field analysis. A possible reason for this discrepancy is suggested by the zero field transmission measurements of Boyle and Rodgers,⁽⁹³⁾ in which they saw a weak absorption edge at about .035 eV*, which could be due to an indirect transition. Since all the data in the zero field experimental curve⁽⁷⁰⁾ were measured at photon energies below .035 eV (See Figure 16), and all of our magnetorefectivity data were measured at photon energies well above .035 eV, it seems reasonable that the relaxation times should be much smaller at the higher photon energies.

* There are several different indirect transitions which could give rise to an absorption edge near .035 eV. It should be noted that at these small energies, the phonon energy must be taken into account. (See the phonon dispersion curves by Yarnell et al., reference 94).

Having achieved a reasonable fit for the lineshape of the $n = 0$ interband transition for one photon energy and sample orientation, we next calculated magnetorefectivity curves for other photon energies and sample orientations, changing none of the parameters of the model. In Figure 18, we show experimental and theoretical curves for a photon energy of .107 eV with the binary sample orientation. Once again a reasonable fit is obtained; even the amplitudes are about correct. The major discrepancy in this case is that the theoretical oscillations are not antisymmetric enough; in particular, the low field sides of the experimental oscillations are much steeper than the low field sides of the corresponding theoretical oscillations. To understand the deficiency of the Lax model which produces this discrepancy, we will discuss the results of another calculation made using the theory of Dresselhaus and Dresselhaus.⁽⁹⁵⁾ In this calculation, a parabolic band model was assumed, (See Section IB) and the parameters of the band model were adjusted to approximate the correct bismuth Landau level energies near $k_H = 0$ for the $n = 1$ and the $n = 2$ Landau levels. It was found that the oscillations predicted by this calculation were much more antisymmetric, and therefore in better agreement with experiment, than are the theoretical oscillations displayed in Figure 18. The key difference between the two models seems to be that the parabolic band model predicts that the Landau level energies are quadratic functions of k_H at large values of k_H , while the Lax model predicts that the Landau level energies are linear functions of k_H at large values of k_H . We therefore conclude that the key deficiency of the Lax model, with respect to the lineshapes of the oscillations under discussion here, is that the Lax model incorrectly gives a linear k_H dependence for the Landau level energies at large values of k_H . This makes sense, since in connection with

our discussion of Figure 14 we noted that we would expect the Lax model to break down at a value of k_H on the order of a few times k_F , and that at large values of k_H , the Baraff terms in the Hamiltonian should dominate, yielding Landau levels with energies which are quadratic functions of k_H .

In Figure 19, we present theoretical and experimental curves for the magnetorefectivity of a sample in the trigonal orientation, using radiation with a photon energy of .1195 eV. Once again we have used the parameters given in Table II. Although the experimental data are not as good as they were previously, due to the small amplitude of the oscillations, we see that once again there is reasonable agreement between theory and experiment. Since the theoretical curves are both a little too sharp, and a little too big, we could probably improve the agreement by decreasing the electronic relaxation times somewhat. This was not done, however, due to the large amount of computer time that would be required.

In summary, therefore, we can state that we have calculated the magnetorefectivity of bismuth for a wide range of photon energies, magnetic fields, and sample orientations using the Lax model and a single set of relaxation times to describe all of the data. We have obtained reasonable agreement between theory and experiment for the interband oscillations, and will present detailed conductivity vs. field curves for the interband transitions in the next part of this section. We have obtained much poorer agreement for the cyclotron resonance oscillation, and will go on to consider these discrepancies in the final part of this section.

CONDUCTIVITY CURVES FOR INTERBAND TRANSITIONS

In this, the third part of this section, we will present conductivity curves for interband transitions associated with the interband oscillations of Figures 17 and 18, where we have obtained reasonable agreement between theory and experiment. We do this at this point for two reasons. First of all, we wish to complete the justification of the arguments of Section IIC, where we have used these conductivity curves to greatly simplify the Baraff model. Secondly, in the final part of this section, where we will discuss the discrepancies between theory and experiment for the cyclotron resonance lineshape, we will find it convenient to present some of our arguments in terms of the conductivity of the material, which can be calculated directly from the band model. It is therefore useful to begin our discussion of the detailed conductivity of the material with the interband oscillations, where reasonable agreement between theory and experiment has been obtained.

In Figures 20a and b, we therefore present curves which describe, as a function of field, the contribution to σ_{-+} from two of the transitions associated with the $n = 1$ interband oscillation. (See Figure 18.) For ease of comparison, we have chosen the photon energies so that the critical field, marked by the dashed line, is 50 kG in each case. We show the real and imaginary parts of the conductivity contributed by a representative spin conserving transition in Figure 20a. The peaks are large and sharp because the velocity matrix element in this case is non-zero at $k_H = 0$, where there is a peak in the joint density of states for the transition. (See Figure 21b.) The large negative peak in the imaginary part of σ_{-+} corresponds to a large peak in the real part of the effective dielectric constant of the material,

according to the notation used in this thesis. Since we are at a photon energy well above the plasma frequency, it is reasonable to find that such peaks give rise to the large peaks observed in the magnetorefectivity of the material.

For the representative spin flipping transition, which contributes to the conductivity as is shown in Figure 20b, we find that the peaks in the conductivity are much smaller and blunter, because in this case, the interband velocity matrix element is zero at $k_H = 0$. As a matter of fact, it is found by direct calculation that the peaks in the conductivity produced by the spin flipping transitions are much too small to produce any observable peaks in the reflectivity.

In Figures 20c and d, we present conductivities for representative transitions associated with the $n = 0$ interband oscillation. This is called the anomalous transition because the nature of the spin flipping and spin conserving velocity matrix elements and transitions are interchanged in this case. (See Figure 21a.) In spite of this peculiarity, however, we note that the shapes of the sharply peaked curves of Figure 20d are quite similar to the shapes of the normal, sharply peaked curves of Figure 20a. We are therefore not able to offer any simple explanation for the difference between the lineshape of the $n = 1$ interband oscillation, which is associated with the transitions of Figures 20a and b; and the lineshape of the "backwards" $n = 0$ interband oscillation, which is associated with the transitions of Figures 20c and d. All we can say is that when we actually work out the calculation, properly including the many effects which we have considered, we correctly predict that the $n = 0$ interband oscillation has the "backwards" lineshape. (See Figure 17.)

Before completing this discussion we should point out that the curves presented here were calculated using the simpler Lax model, rather than the more accurate Baraff model. We showed in Section IIIE, however, that there is no large, zeroth order difference between the Baraff and Lax velocity matrix elements or Landau level energies for the interband transitions under discussion. It therefore seems reasonable to assume that the curves we have just presented are reasonably accurate. In the next part of this section, however, we will discuss the cyclotron resonance oscillation, where the Lax model does not seem to be accurate at all.

CYCLOTRON RESONANCE LINESHAPE

In this, the final part of the section, we will discuss the large discrepancies between the measured lineshape of the cyclotron resonance oscillation and the lineshape calculated from the Lax model. These discrepancies are illustrated in Figures 5 and 17. From these figures we see that the major difficulties with the theoretical curves are: a) that the shoulder which occurs just above the cyclotron resonance critical field is insufficiently sharp; and b) that the dip in the reflectivity which occurs just below the cyclotron resonance critical field is much too deep.

These deficiencies of the model of Lax and Wolff can be understood by considering the more accurate model of Baraff. First of all, in Figure 21a, we note that there is a large difference between the Baraff and Wolff velocity matrix elements for the cyclotron resonance (intraband) transition. In particular we note that the Baraff spin conserving intraband velocity matrix element is much more sharply peaked in the vicinity of $k_H = 0$ than is the corresponding Wolff velocity matrix element. We believe that it is this

inaccuracy in the Wolff velocity matrix element which leads to the inadequate sharpness of the theoretical cyclotron resonance oscillation. The reason for this is that the cyclotron resonance oscillation, like the other oscillations which we have discussed so far, is associated with a peak in the joint density of states at $k_H = 0$ for an inter-Landau level transition which is allowed at $k_H = 0$ (in this case, the $j = 0$ to $j = 1$ spin conserving intraband transition.) The sharp peak in the Baraff velocity matrix element for the spin conserving intraband transition would tend to emphasize even further the contribution to the conductivity due to transitions with small values of k_H , effectively increasing the sharpness of the peak in the joint density of states at $k_H = 0$. It therefore seems reasonable to assume that the use of the more accurate Baraff model would correctly lead to a theoretical magnetorefectivity curve with a sharper shoulder for the cyclotron resonance line; and that therefore it is the inaccuracy in the Wolff velocity matrix element which leads to the inadequately sharp cyclotron resonance oscillation predicted by our calculation.

We will next consider the large dip in the magnetorefectivity which occurs at fields which are greater than the $n = 0$ interband oscillation critical field, but are lower than the cyclotron resonance critical field. Using Figure 14, we see that for these fields,* the Lax model predicts that: a) the photon energy will be too small for any interband transition; and b) the photon energy will also be too large for any intraband transition.

* In Figure 14, we show the Landau level energies for a field of 50 kG along the binary axis. If we did a magnetoreflexion experiment at a photon energy of .065 eV, 50 kG would fall in the range of fields under consideration.

Therefore, the Lax model predicts that the light ellipsoids will contribute essentially no losses for this range of fields. It is this sudden decrease in the real part of the conductivity which makes the dip in the reflectivity under consideration much too large.

In contrast to the Lax model, the Baraff model does not predict such a sudden dip in the real part of the conductivity. The reason for this is that the Baraff interaction decreases the critical field for the spin flipping intraband transition so that it is still possible to make an energy absorbing, spin flipping $k_H \neq 0$ intraband transition at a field in the range under consideration. It therefore seems reasonable to assume that the inclusion of the additional energy losses predicted by the Baraff model would decrease the size of the calculated dip in the magnetorefectivity.

To check out this assumption, we have re-done the calculation of Section IIID, modifying the results obtained there so as to take into account, in a crude way, the Landau level energy shifts produced by the Baraff interaction. Essentially, we first approximated the Baraff expressions for the Landau level energies by neglecting the k_H dependence of the Baraff correction terms, and then substituted these energy expressions into the resonance denominators of Eqs. IIID77 and 80. We found that as a result of these modifications the magnitude of the dip in the reflectivity was reduced by approximately 50%, and that much better agreement between theory and experiment was obtained. We therefore conclude that the reason that the Lax model yields much too large a dip in the magnetorefectivity just below the cyclotron resonance critical field is that this model neglects the shift in the critical field for the spin flipping intraband transition produced by the Baraff interaction.

Up to this point, we have been emphasizing the discrepancies between the predictions of the Lax model and the experimentally determined cyclotron resonance lineshape. It should be pointed out, however, that the Lax model is in agreement with experiment in predicting that the cyclotron resonance line has a shoulder-like lineshape. To understand this from a more physical point of view, we make use of Figures 20e and f, where we show the contributions to the conductivity due to the transitions associated with the $n = 0$ intraband oscillation (the cyclotron resonance oscillation,) calculated using the Lax model. These curves have several interesting features. First of all, since these transitions are normal ones, the contribution to the conductivity from the spin conserving transition is much larger than the contribution from the spin flipping one. Secondly, the real part of the conductivity for the spin conserving transition displays a broad plateau rather than a sharp peak. The reason for this broad plateau is that this transition can absorb energy for a broad range of fields above H_{cr} since the energy required to make this transition decreases with increasing k_H . (See Figure 14.) The cutoff field, H_{co} , is the maximum field at which energy can be absorbed by a direct intraband transition, and is equal to the field at which the photon energy is identical to the energy required to make a $j = 0$ to $j = 1$ intraband transition at $k_H = k_F$, where k_F is the value of the crystalline momentum along the magnetic field at which the $j = 0$ Landau level passes through the Fermi level. As required by the Kramers-Kronig relations, a negative peak in the imaginary part of the conductivity is also predicted at H_{co} .⁽⁴⁴⁾

From the preceding comments it seems that the physical reason there is a shoulder in the reflectivity at H_{cr} is that at fields above this field there

is a sudden increase in the losses of the material. This reasoning also predicts that there should be another shoulder at H_{co} , where the reflectivity of the material should suddenly drop, and upon carrying out the detailed calculation, this is found to be the case. This second shoulder has an amplitude of about 10% of the zero-field reflectivity, and is not shown in Figure 17 only because it occurs at fields well above 100 kG.

The second shoulder is very troublesome, however, because though the theory predicts that it should be easily observable at lower photon energies, occurring at fields below 100 kG with an amplitude of 5-10%, no such oscillations have ever been observed in the reflectivity. On the contrary, we find that the reflectivity remains relatively constant at fields above the cyclotron field, right up to the highest fields we can obtain. Similar difficulties were uncovered in the far-infrared cyclotron resonance studies of Hebbel and Wolff.⁽⁴⁴⁾ On the basis of a simple Kramers-Kronig argument, they also predicted that there should be an oscillation in the reflectivity at the field H_{co} . In common with our experiments, no such oscillation was ever observed. We have no explanation for this interesting discrepancy,* but clearly something very peculiar is going on at the Fermi surface of the material.

*It should be emphasized that no conceivable band structure can completely explain this discrepancy. First of all, if the band structure predicts that the energy required to make intraband transitions is a function of k_H , a calculation such as the one given in this thesis will always predict that there should be two shoulders in the reflectivity. If, on the other hand, the energy required to make intraband transitions is not a function of k_H (i.e. parabolic bands,) then $H_{cr} = H_{co}$ and one finds that the two shoulders associated with these fields should overlap, giving rise to a large peak in the reflectivity. Such a theoretical result also disagrees with experiment.

At this point we would normally finish the discussion by using the theoretical calculation to find an easily recognizable feature of the cyclotron resonance lineshape which closely corresponds to the critical field for the oscillation, and in this way develop an experimental definition for the resonance field. In particular, Figure 17 shows that the critical field for the cyclotron resonance oscillation is most closely associated with the steepest part of the oscillation lineshape. Therefore, in analyzing the data in Section IIC we have defined the cyclotron resonance field as the field at the steepest part of the cyclotron resonance lineshape. In view of the difficulties discussed in this part of this section, our confidence in this definition is rather low, and we have not attempted to evaluate any of the band parameters using the cyclotron resonance data. It is interesting to note, however, that in Figures 6 and 10, good agreement is still obtained between theory and the experimental data.

CHAPTER IV

ARSENIC

Recent experimental and theoretical studies of the semi-metal arsenic have greatly advanced our understanding of the band structure of this material. In particular, Lin and Falicov⁽¹²⁾ have calculated the band structure of arsenic using a pseudopotential technique and have obtained a Fermi surface whose shape is in reasonable agreement with a large body of experimental data. Since almost no experimental information was available about the band structure away from the Fermi level, we therefore felt it would be interesting to study arsenic using the magnetoreflexion technique, which gives such information, and use our experimental results to explore the validity of the Lin-Falicov model away from the Fermi surface. Our study has been quite successful, and we have several new findings to report.

In Section A of this chapter we will discuss the experimental and theoretical studies which have preceded our work. In Section B we will describe the techniques we used to prepare our samples. In Section C we will discuss the information which can be extracted from magnetoreflexion experiments performed with the field parallel to the binary and bisectrix axes. In Section D we will discuss the experiments performed with the magnetic field parallel to the trigonal axis. Finally in Section E, we will summarize our results, and present some suggestions for future experiments.

SECTION IVA

BACKGROUND MATERIAL

WORK PRECEEDING THE BAND MODEL OF LIN AND FALICOV

The first really detailed information about the band structure of arsenic was obtained in a set of DHVA experiments performed in 1955 by T.G. Berlincourt.⁽⁷⁸⁾ Two sets of carriers were observed which we will call the α and γ carriers, using the notation* of Lin and Falicov.⁽¹²⁾ The α carriers were found to lie in either three or six pockets, with the center of each pocket in one of the mirror planes. The γ pockets had a much smaller cross sectional area than the α pockets, and their number and placement in the Brillouin zone were not completely clear. The effective masses were found by studying the temperature dependence of the amplitude of the DHVA oscillations. In Table III we present values for the carrier effective masses and cross sectional areas as measured by a number of experimentalists, Berlincourt among them, along with those theoretical values calculated by Lin and Falicov.

Since the total hole and electron charge concentrations must be equal in a pure semimetal, the results of Berlincourt indicated that there was at least one more carrier yet to be found. De Haas-van Alphen type oscillations in the ultrasonic attenuation and differential susceptibility, observed in 1965 by Shapira and Williamson,⁽⁷⁹⁾ were identified with this carrier, which we will call** the β carrier, using the notation of Lin and Falicov. The comments made about the number and orientation of the α pockets apply equally

* Berlincourt used a different notation himself. Our γ and α carriers correspond to his α and β carriers, respectively.

** This was called the γ carrier by Shapira and Williamson. For the other two carriers, they used the notation of Berlincourt.

well to the β pockets. In addition, the β pockets were found to be roughly ellipsoidal in shape, while the α pockets displayed some non-ellipsoidal behavior. The temperature dependence of the oscillations was not reported, so no information about the effective masses was obtained. Ketterson and Eckstein⁽⁸⁰⁾ also carried out an ultrasonic magnetoattenuation experiment, obtaining results consistent with the work of Shapira and Williamson. They also did not measure the temperature dependence of the oscillations.

In 1965, an attempt was made by Tanuma⁽⁸¹⁾ et al. to identify the sign of the charge for the α , γ , and β carriers by studying the effect of doping on the DHVA periods. The results, however, were inconclusive.

Finally in 1965, Datars⁽⁸²⁾ studied arsenic using Azbel-Kaner cyclotron resonance in the extreme anomalous limit. The cyclotron effective masses he measured agreed reasonably well with those found by Berlincourt⁽⁷⁸⁾ for the α carriers.

BAND MODEL OF LIN AND FALICOV

In 1965, Lin and Falicov⁽¹²⁾ published the results of a pseudopotential calculation of the energy bands for arsenic, which have served as a guide to the interpretation of all the subsequent work. In such a calculation, one replaces the rapidly varying part of the crystalline potential near the atomic nucleus with a smooth pseudopotential which has several adjustable parameters. One then adjusts these parameters to fit the experimental information available about the band structure. Lin and Falicov did not consider the effects of the spin-orbit interaction in their calculation, and since they were mostly concerned with the general topology of the Fermi surface, they fit their model to the available DHVA⁽⁶⁾ data.

They identify the β carriers as electrons, which lie in three roughly ellipsoidal pockets centered about the L points in the Brillouin zone. The α and γ carriers correspond to parts of the multiply connected hole surface shown in Figure 22. The α carriers lie in the six large turnip shaped pockets, and the γ carriers are in the long, narrow necks which connect them. Note that though the holes lie near the T point, there are no carriers at T, or in fact, anywhere along the TT' , or trigonal axis. In Figure 23a we show a particularly interesting portion of the band structure which was used to construct the Lin-Falicov Fermi surface. In this figure we see that along the TW , or binary axis, close to T, there is an accidental cross over degeneracy. The Fermi level cuts the bands just below the degeneracy, giving rise to the hole carriers of the γ necks. If spin orbit coupling had been considered, this degeneracy would be split, as shown in detail in Figure 23b.

The only symmetry operation at a general point along the TW or Q axis is a two-fold rotation about this axis, so that, lacking inversion symmetry,

the extrema of the two bands need not occur at the same point, and the energy gap, E_g , will be at the point of minimum energy separation, as shown. We have observed oscillations in the magnetorefectivity which may be associated with interband transitions across this spin-orbit energy gap.

The band structure of arsenic was also calculated by Golin in 1965, using a self-consistent OPW method.⁽⁸³⁾ His results are very similar to those of Lin and Falicov insofar as the gross features of the band structure are concerned. No fit to the experimental data at the Fermi surface could be achieved with Golin's bands, however. This is to be expected, since his estimated error is greater than one of our observed energy band gaps.

The detailed DHVA studies made recently by Priestly et al.⁽⁶⁾ and Vanderkooy and Datars⁽⁹⁶⁾ have tended to support the general topology of the Lin-Falicov band model, as do the Azbel-Kaner cyclotron resonance studies of Datars and Vanderkooy,⁽⁹⁷⁾ and Chung-Sen Ih.⁽⁷⁾ However, the effective masses which they measure are quite different from those predicted from the model,⁽¹²⁾ leading one to believe that the model may not be accurate away from the Fermi surface. Therefore, optical data would be of great interest.

Unfortunately only one set of optical experiments have been carried out on arsenic. This work was done by Cardona and Greenway⁽⁸⁴⁾ in 1964, in the photon energy range between 1 and 23 eV, using unpolarized light reflected from a cleaved trigonal face in zero magnetic field. There was, therefore, a nearly complete lack of optical information in the infrared, which is the region most likely to contain detailed information about the band structure near the Fermi surface. We will present our zero field and magnetorefectivity measurements, which explore precisely this region, in Sections VIC and D.

SECTION IVB

SAMPLE PREPARATION

Arsenic is a far more difficult material to work with than is bismuth. First of all the crystals are much harder to grow, since arsenic sublimates at 615°C and does not melt until a temperature of 817°C and a pressure of 36 atmospheres are reached.⁽⁸⁵⁾ Also, it may crystallize in many allotropic forms.⁽⁷⁸⁾ Secondly, when we began our experiments there were no known ways to achieve a strain free, highly polished optical binary or bisectrix face, though trigonal faces of adequate quality had been prepared by cleaving.⁽⁸⁴⁾ Finally, the material is quite reactive, and must be carefully protected from the atmosphere to keep the optical surfaces from oxidizing.⁽⁷⁾ The oxide, of course, is highly poisonous.

The single crystal boules were grown in a quartz bomb under high pressure by a modified Bridgeman technique,⁽⁸⁵⁾ and had a resistivity ratio, $R_{300^{\circ}\text{K}}/R_{4.2^{\circ}\text{K}}$ of more than 300.⁽⁷⁾ The material was kept coated with clear Krylon whenever it was not being processed. When protected in this way samples showed no oxidation after being stored for more than one year.

The boules were cleaved, X-rayed and oriented using the same techniques as were used to make the bismuth samples. They were then spark cut and the binary and bisectrix optical faces were chemically polished. Difficulty was encountered with the highest quality samples during these two steps, since the material was sufficiently free of strain and impurity hardening that it cleaved during the cutting and polishing operations. It was found that by sandwiching the samples in between pieces of GaAs during the cutting and polishing operations, good results could be obtained.⁽⁸⁶⁾

The chemical polishing was done with a 1% chlorox solution. A high nap polishing paper was used on the polishing wheel, and the weight of the sample holder was supported by three GaAs spacers which rested upon the wheel. As the polishing progressed the GaAs was dissolved by the solution so that the sample was fed into the wheel at a slow uniform rate, while most of the mechanical stresses were taken up by the GaAs spacers.

The samples were mounted in the dewar in the usual way. The Krylon was removed with an acetone soaked cotton swab just before the vacuum was applied.

SECTION IVC

RESULTS FOR BINARY AND BISECTRIX FACES

The experimental magnetoreflexion results obtained with the magnetic field parallel to the binary and bisectrix axes were very similar. In Figure 24 we first display a representative experimental trace taken with the magnetic field parallel to the binary axis. The oscillations are quite small as compared with the oscillations observed in other semimetals, so that many sweeps with the Enhancetron were required. Furthermore, the lineshape does not display any sharp structure so that it is not clear what feature of this lineshape corresponds to the critical field, as defined in Section IA. If the photon energy of .410 eV at which this curve was observed were well above the plasma frequency, then it would be reasonable⁽²⁸⁾ to assume that the reflectivity peak corresponds to the critical field; however, no value for the plasma frequency of arsenic has been quoted in the literature. We therefore measured the zero field reflectivity of arsenic for $\vec{E}$ both parallel and perpendicular to the trigonal axis. The results are shown in Figures 25 and 26.

Our equipment is not well suited for making zero field measurements of this type, so the curves displayed have only qualitative validity. To make these measurements the magnet was removed, an aluminum mirror was mounted on the outside of the dewar, and a mechanical servo system was used to place first the mirror, and then the sample, into the aperture of the optical system. The amplitude of signal observed when the mirror was in the light beam was set to 10.5 arbitrary units by adjusting the amplifier gain, and then, without resetting the gain, the amplitude of the signal observed with the sample in

the beam was recorded. During these measurements, the sample was kept at liquid helium temperatures.

The plasma frequencies are very close to the frequencies at the reflectivity minima,⁽⁸⁷⁾ which were measured to be .30 and .26 eV for $\vec{E}$ parallel and perpendicular to the trigonal axis, respectively. The frequency at which the oscillations of Figure 24 were observed is well above the plasma frequency for both polarizations, so we may assume⁽²⁸⁾ the critical field corresponds to a resonant field which we experimentally define as the field at the peak in the reflectivity. Note that these oscillations have nothing to do with the peak in the zero field reflectivity of Figure 26 labeled "Interband Transition," which will be discussed in more detail in Section D.

All the other oscillations observed with the magnetic field parallel to the binary axis are also observed at photon energies well above the plasma frequency, so we may use this experimental definition of the resonant field for them all. When we plot these resonance fields as a function of photon energy, the fan chart of Figure 27 is obtained. For photon energies near the gap of 0.346 eV, the spacing of the lines is what one would expect for nondegenerate parabolic bands with no spin-splitting, and a reduced effective cyclotron mass of 0.023. The integers, n , label the interband transitions in accordance with such a simple model. At higher energies the lines become decidedly curved indicating that the energy bands are no longer described by parabolic dispersion relations.

It was found that the amplitude of the oscillations depended upon the polarization of the light. This effect was exploited in order to get some information about the placement in the Brillouin zone of the critical point associated with the corresponding interband transition. It was found that

the oscillations were extinguished when the light was polarized perpendicular to the trigonal axis. This implies that the component of the interband velocity matrix element perpendicular to the trigonal axis is zero, and the component parallel to the trigonal axis is nonzero. To use this information,⁽⁴⁾ one now looks at the high symmetry points in the Brillouin zone,⁽⁶⁷⁾ and tries to find a pair of bands which have the proper symmetry such that these selection rules will hold. The critical point may then only be at a point in the Brillouin zone where such a pair of bands may be found. In our case, the critical point must lie on the $\Gamma\Gamma$, or Λ axis, where the point Γ is at the center of the Brillouin zone (See Figure 1). In the notation of Lin and Falicov, these transitions can occur only between bands of the symmetries:

$$T_1 \quad \text{and} \quad T_2',$$

$$T_1' \quad \text{and} \quad T_2,$$

$$\Gamma_1 \quad \text{and} \quad \Gamma_2',$$

$$\Gamma_1' \quad \text{and} \quad \Gamma_2,$$

$$\Lambda_1 \quad \text{and} \quad \Lambda_1,$$

$$\text{or} \quad \Lambda_2 \quad \text{and} \quad \Lambda_2.$$

Thus the polarization experiment gives information not only about the location of the critical point in the Brillouin zone, but also about the band ordering near the Fermi level.

If the oscillations are due to interband transitions with a critical point along the Λ axis, then due to the threefold rotation symmetry about this axis, the same fan chart should be observed for the bisectrix face at low

fields and photon energies where the parabolic band model is still valid. In Figure 28 we show the oscillations observed with the magnetic field parallel to a bisectrix axis for a photon energy of 0.412 eV. The resonant fields are plotted as circles on the fan chart of Figure 29. The triangles are from the oscillations observed for the binary face, but plotted on the same figure for comparison. The agreement of the resonant frequencies between the two faces is excellent.

Although the fan charts for the two faces are in good agreement, the lineshapes in Figures 24 and 28 are somewhat different. This is to be expected, since the contribution to the conductivity from the other carrier pockets may be different for the two orientations. In addition to this inherent differences there is an instrumental one as well, in that the binary data were taken with the prism monochromator, and the bisectrix, with the grating monochromator.

Data were taken at only one photon energy above the region of atmospheric absorption, because of the poor signal to noise ratio at these photon energies. Even though the binary data show considerable deviations from a simple parabolic band model in this region, the binary and bisectrix data still agree very well. Any discrepancies between the two sets of data may be attributed to the differences in the lineshapes. The bisectrix data can be fit by a spinless parabolic two-band model, with a reduced effective cyclotron mass of .026, and an energy gap of .346 eV. Note that the $n=0$ line is observed for the bisectrix face. The probable reason it was not observed for the binary face is that the smaller resolution of the prism instrument, used for those experiments, broadened this oscillation to the point where it could no longer be seen.

The position of the critical point for the interband transition we have been discussing can be pinned down even further, by using the same argument that was used to show that the electrons in bismuth are at the L point in the Brillouin zone. Once again the simplicity of the spectrum observed implies that the two-band extrema are at the same point in the Brillouin zone,⁽³¹⁾ which implies in this case that the extrema are at T, where this coincidence is required by symmetry. The Γ point is ruled out by the band calculations discussed in Section IA,^(14-16,83) which show that there are no small band gaps at Γ .

In Figure 30 we show the relationship between the photon energy and the amplitude of the $n=0$ oscillation, as observed for the bisectrix face. The amplitude goes to zero for a photon energy of .360 eV, which is .014 eV above the energy gap. A similar cutoff was also observed in the binary data, but not quite as clearly, because the $n=0$ curve, where the effect is most pronounced, was not observed in that case.

Generally such a cutoff implies that the Fermi level lies within one of the bands associated with the interband transition, and not in the energy gap between them.⁽⁴⁾ This is because each of our oscillations corresponds to a transition between Landau levels in two different bands, and will be extinguished below that photon energy at which one of the Landau levels has passed through the Fermi level, so that both Landau levels are either occupied or unoccupied.

In summary, therefore, we conclude that in arsenic there is a very small pocket of carriers in addition to those already observed. This additional carrier is centered about point T in the Brillouin zone, and its dispersion relation is still parabolic at energies considerably above the Fermi energy.

There is an allowed transition between this band and another band separated by an energy gap of .346 eV, provided that the electric field is not perpendicular to the trigonal axis. Since the only component of the velocity matrix element between these bands is parallel to the trigonal axis, the f-sum rule for effective masses⁽²⁸⁾ indicates that the component of the effective mass tensor parallel to the trigonal axis is probably a lot smaller than the component perpendicular to it, so that the Fermi surface for this carrier is an oblate ellipsoid of revolution. The reduced cyclotron effective mass for magnetic fields perpendicular to the trigonal axis is $0.025 \pm .002$. An explicit value for the Fermi level may not be determined without knowing details of the band structure, such as the spin splitting of the Landau levels. Such detailed information is not available.

Oscillations due to this additional carrier have never been observed by DHVA or Cyclotron Resonance techniques. This is reasonable, because the DHVA period for this carrier could be very long and difficult to observe, and the number of carriers involved is probably quite small. We may also argue that since the Fermi energy and effective masses seem to have the same order of magnitude as do the corresponding quantities for the γ necks,⁽⁶⁾ the number of carriers in the two types of pockets are also on the same order of magnitude, so that the number of carriers in our new pocket is much too small to affect charge compensation. We cannot calculate these quantities from our data, however, since we know only one reduced effective mass, and have only a reasonable guess for the Fermi level.

The Lin-Falicov⁽¹²⁾ band model displays no such carrier since it was fit to available DHVA⁽⁶⁾ data which displays no oscillations which may be identified with it. A more serious difficulty with this model, however, is

the lack of any small energy gap along the Λ axis between bands of proper symmetry, as determined by our experiments. Since the experimental situation is quite unambiguous, it is hoped that the pseudopotential parameters may be varied to bring the calculated band structure into agreement with our data.

SECTION IVD

RESULTS FOR THE TRIGONAL FACE

When the magnetic field is placed parallel to the trigonal axis, the oscillations which are observed in the magnetorefectivity of arsenic are larger than the oscillations observed in any other semimetal.⁽³⁻⁵⁾ Three representative experimental traces measured at liquid helium temperatures are displayed in Figure 31. One reason for the large amplitude of these oscillations is that we are at a frequency near the plasma frequency (See Figure 26) where the free carrier contribution to the conductivity is nearly cancelled out by the contribution due to the core polarization, so that any oscillatory effects in the conductivity are greatly enhanced.⁽⁸⁸⁾ Other reasons for the large magnitude of these oscillations will shortly be discussed.

Although we have found these oscillations easy to observe experimentally, we have found it impossible to understand their complicated lineshape in terms of any available lineshape calculation. We have therefore developed a model which is capable of explaining the essential features of our experimental results. Since it is convenient to have a theoretical framework available when discussing experimental data, we will first briefly present this model on a purely a priori basis, and then show it is applicable to the data under discussion by comparing its predictions with experimental observations. The model is discussed in much greater detail in Appendix A.

First of all, we postulate that the oscillations of Figure 31 are due to interband transitions between two non-degenerate* bands with essentially quadratic dispersion relations. These interband transitions produce the oscillation in the zero field reflectivity shown in Figure 26. Due to the parabolic nature of these bands, the usual Landau level structure will be obtained** in the presence of a magnetic field. Secondly, we assume that the curvatures of the two bands in the x(binary) direction are large, equal and opposite, and that the same is true of the band curvatures in the y(bisectrix) direction. In the z(trigonal) direction, however, we assume that the band curvatures are small, so that the constant energy surfaces for the bands are elongated in the z direction. We will further assume that these elongated constant energy surfaces are tilted from the trigonal axis by a small amount, but that the tilts for the conduction and valence bands are not equal, so that these constant energy surfaces are also tilted with respect to each other. Finally, we will assume that the energy extrema for the two bands are nearly coincident.

Let us now consider the selection rules for interband transitions between two such bands. Placing the magnetic field in the z direction, where the extrema are nearly coincident, we see that at $k_z = 0$ we will be making transitions between two nearly concentric, similar, ellipsoidal orbits.

* Due to the low symmetry of the A7 crystal structure, all band degeneracies are removed when spin-orbit coupling is considered. (67)

** For simplicity, the effects of spin on the Landau levels will be ignored.

Therefore the usual selection rule, $n = n'$, will apply, where n and n' refer to the Landau level indices of the two orbits involved in the interband transition.⁽²⁸⁾ When $k_z \neq 0$, however, the two orbits will be displaced with respect to each other due to the relative tilt of the constant energy surfaces, and the simple selection rule will break down. (See Appendix A.) Therefore, when $k_z \neq 0$, transitions will be allowed between Landau levels of any n and any n' .

Using these k_z dependent selection rules, we may now calculate $\epsilon(n, n')$, the contribution to the dielectric constant from interband transitions between Landau levels of indices n and n' . This calculation shows that at a high enough photon energy, the tensor $\epsilon(n, n')$ will display a peak in both its real and imaginary parts when the magnetic field is approximately equal to $H_c(n, n')$, where $H_c(n, n')$, the critical field for the transition under discussion, is defined* by the equation

$$\hbar\omega = E_g + \frac{\hbar e H_c(n, n')}{m_0 c m_c^*} (n + n' + 1), \quad (\text{IVD1})$$

where $\hbar\omega$ is the photon energy, E_g is the energy gap, and m_c^* is the ordinary one-band cyclotron effective mass. We may next define the total index number, n_t , as

$$n_t = n + n', \quad (\text{IVD2})$$

* This definition of the critical field is essentially equivalent to the one given in Section IB.

and conclude from Eq. IVD1 that all transitions with the same total index number will have the same critical field, and therefore all such transitions will contribute to a single oscillation in the reflectivity. Finally, since the major contribution to the n_t -even oscillation comes from the $n = n'$ transition, we can conclude that the only additional oscillations which will be observed due to the breakdown of the selection rules are those oscillations with odd values of n_t .

We next would like to compare the lineshape of the oscillations predicted by the model we have been discussing with those experimentally observed. The most straightforward way of doing this, of course, would be to do a line shape calculation similar to the one we have carried out for bismuth. As is pointed out in Appendix A, such a calculation would be extremely difficult, since it would take an enormous amount of time to sum over a sufficient number of transitions. We have therefore taken a much less rigorous approach, and will merely compare some of the essential features of the experimental and theoretical oscillations.

This comparison is greatly simplified by assuming that the photon energies at which our measurements were made exceed the plasma frequency by a sufficient amount so that the lineshapes of the oscillations are not distorted by plasma effects. This is equivalent to assuming that we are in the high frequency limit where the lineshape of each oscillation in the reflectivity is similar to the lineshape of the corresponding oscillation in the real part of the total effective dielectric constant. Since we are close enough to the plasma frequency for the overall amplitude of our oscillations to be strongly enhanced by plasma effects, this assumption requires some justification. To demonstrate its validity, we first note that a lineshape distortion induced by a plasma

effect would be strongly photon energy dependent. Furthermore, we note that for a particular value of n_t , the lineshape of the observed oscillations is essentially independent of the photon energy; changing the photon energy seems only to change the field and reflectivity scales of the magnetorefectivity curves, so that no such strongly photon energy dependent distortions are observed. We may therefore conclude that our assumption is correct, and that we are in the high photon energy limit above .190 eV, which is the lowest photon energy at which the lineshape of the oscillations can clearly be seen.

We are now ready to discuss the oscillations of Figure 31. First of all, using the argument of the preceeding paragraph, we conclude that the peak in the reflectivity coincides with the peak in the dielectric constant, and that, therefore, the field at the peak in the reflectivity is approximately equal to the critical field. We have therefore experimentally defined the resonant field as the field at the peak in the reflectivity, and labeled each of the peaks in Figure 31 with its associated total index number, n_t . It will be noted that the amplitude of these oscillations is a strong function of n_t . In particular, the amplitude of the n_t -even oscillations decreases with increasing n_t much more rapidly than does the amplitude of the n_t -odd oscillations.* From the explanation we have given for their origin, it is not surprising that the n_t -even and the n_t -odd oscillations display quite different characteristics, and upon estimating the relative amplitudes of these oscillations, we find

* The n_t -even oscillation amplitudes decrease so rapidly with increasing n_t , that we were not able to clearly observe the $n_t = 6$ oscillation at all. This oscillation was observed, however, in a high resolution magnetoreflexion experiment, using a laser source, performed by Dr. S. Iwasa of the M.I.T. Physics Department. (89)

that our theory gives qualitative agreement with experiment. In Appendix A we have gone into this complicated matter in some detail, and will therefore not repeat this discussion here.

We will, instead, consider the dependence of the resonant fields upon the photon energy, and will be able to show, in a relatively straightforward way, that almost all of the assumptions which we made in setting up our model can be justified on the basis of this information alone. We therefore begin by plotting the resonance fields as a function of photon energy in the fan chart of Figure 32. Looking at this figure, it is clear that our oscillations are associated with interband transitions across a single band gap of about .175 eV. Furthermore, the lines on this fan chart are relatively straight, so that we can assume that the energy bands are relatively parabolic at the energies where we have been able to observe the oscillations. From this fan chart, we could also estimate a value for m_c^* . There is, however, another more accurate and more instructive way of processing the data.

First of all, from Eq. IVD1, we expect that, when the photon energy is held constant, the oscillations should be periodic in $1/H$ with a period, P , given by the equation

$$P = \frac{\hbar e}{m_o c m_c^* (\hbar \omega - E_g)} , \quad (\text{IVD3})$$

and a phase of -1 .^{*} In Figure 33, we have therefore plotted the inverse resonant fields as a function of n_t for the data of Figure 31, and we see

^{*} This phase is usually (bismuth, arsenic with $H \perp$ trigonal axis) equal to $-1/2$.

that the points do fall on straight lines with an n_t intercept of -1. Upon closer inspection, it will be noted that most of the very small experimental scatter is due to a systematic shift of n_t -odd oscillations to higher resonant fields, which is probably due to a small difference between the lineshape of the n_t -even and n_t -odd oscillations. The agreement, therefore, is very good.

Secondly, from Eq. IVD3, we see that $1/P$ should be a linear function of the photon energy, with a slope of

$$\frac{2(1/P)}{2(\hbar\omega)} = \frac{m_o m_c^*}{\hbar e} \quad (\text{IVD4})$$

and an energy axis intercept of E_g . We have therefore, plotted in Figure 34 the photon energy as a function of $1/P$ for all of the data we have obtained. Fitting the low energy data with a straight line, we obtain an energy gap of about .177 eV, and from the slope of the line we find that m_c^* is about .031. At higher photon energies the departure of the points from the straight line indicates that the bands have a small, but noticeable amount of nonparabolic character.

The small value we have found for m_c^* indicates that the two bands under consideration interact strongly with each other in the x and y direction. In these directions, it therefore seems reasonable to assume that we may neglect the interaction of our two bands with the other bands nearby,* which implies that the band curvatures will be equal and opposite in the x and y directions, as we have assumed in setting up our model. The assumption that the two

* This is not true along the z direction, where we will find that the two bands interact very weakly with each other.

bands interact only with each other, however, is the essential assumption made in setting up the^(25,35) Lax two-band model, and therefore can be checked by seeing if the nonparabolic nature of the bands can be properly described by this model.

We may show, from Eqs. IB8 through 10, that in the limit where $E_g \gg \beta^* H$, that, for the Lax model

$$\beta^* \frac{1}{P} = \frac{(\hbar\omega)^2 - (E_g)^2}{2E_g} \quad (IVD5)$$

We have therefore plotted $(\hbar\omega)^2$ as a function of $1/P$ in Figure 35. We find that the data does fall on a straight line, justifying the assumption of a two-band model for the x and y directions. From the $(\hbar\omega)^2$ intercept we find that $E_g = .172$ eV, and from the slope of the line we obtain $\beta^* = 4.87 \times 10^{-4}$ eV/kG. This is probably the most accurate value for E_g . In this model, the one band cyclotron mass, m_c^* depends upon the energy, according to the equation

$$m_c^* = \frac{1}{\beta^*} \frac{e\hbar}{m_0 c} \frac{2E}{E_g} \quad (IVD6)$$

and is .0238 at the bottom of the band, where $E = E_g/2$.

Upon comparing these results with the DHVA and cyclotron resonance measurements which have been reported in the literature, (See Table III), we note that this is an uncharacteristically large band curvature for arsenic. As a matter of fact, the only values of m_c^* which have been reported that are anywhere near this small are the values measured for the γ carrier with the magnetic field along the trigonal direction. Using the Fermi level reported by Priestly,⁽⁶⁾ (.011 eV away from the band edge) and Eq. IVD6, we would

predict a value of .0269 for m_c^* if we assumed that the holes of the γ necks were associated with one of the bands we have been discussing. Since this value agrees very well with the value of .028 measured by Priestly, it seems very reasonable to assume that one of our bands is, in fact, associated with these carriers.

Since there are carriers associated with one of the bands, we have looked for a Fermi level cutoff similar to the one observed for the binary and bisectrix data. Unfortunately, however, we have not been able to decide whether or not such a cutoff exists. The essential difficulty is that we were no longer able to see any sharp structure in the reflectivity at photon energies below .190 eV due to the finite resolution and signal to noise ratio of our instrument. Therefore, though we can be sure that there is no cutoff above this photon energy, we cannot be sure that there is no cutoff below it. The reason why this difficulty arises in spite of the very large amplitude of our oscillations can be understood by looking at Figure 31a. In this figure, it can be seen that the $n_c = 0$ and the $n_c = 1$ oscillations overlap to give us a reflectivity curve with no really sharp structure associated with the $n_c = 0$ oscillation. The sharp dip between the $n_c = 1$ and the $n_c = 2$ oscillations, on the other hand, occurs at relatively low fields, so that it fades into the noise at the relatively high photon energy of .190 eV, and below this photon energy we can observe no sharp structures in the magneto-reflectivity at all. Although we cannot tell, from our data, whether or not there are carriers associated with the bands under discussion, we can make the statement that if there are carriers, their Fermi level does not greatly exceed .018 eV, which is the difference between the energy gap of .172 eV and the photon energy of .190 eV, above which the oscillations may be clearly

observed. Therefore the Fermi level of .011 eV, measured by Priestley,⁽⁶⁾ is consistent with our data.

Many of the other characteristics of the γ carriers are also consistent with our data. For example, Priestley finds that the Fermi surface for these carriers is a gently flared cylinder, with the long axis of the cylinder tilted about 11° away from the trigonal axis in the trigonal-bisectrix plane. The curvature of this band in the z direction is therefore very small, and the cyclotron effective mass is very large when the magnetic field is parallel to the binary or bisectrix axes. The small band curvature would give us a very high density of states in the z direction which agrees with the large magnitude of our observed oscillations; and the large effective cyclotron masses agree with our inability to observe any oscillations associated with these bands for the binary and bisectrix sample orientations. We therefore conclude, on the basis of both magneto-optical and DHVA⁽⁶⁾ data, that the bands under consideration have constant energy surfaces which are greatly elongated in the z direction, as was assumed in setting up our model. Furthermore, this small band curvature implies that the bands do not interact strongly with each other along the z direction, so that one would expect the constant energy surfaces to be tilted with respect to each other, unless the bands were at a point of high symmetry. The 11° tilt angle of the carriers⁽⁶⁾ rules out this possibility, so that we can also conclude that the constant energy surfaces of the two bands are tilted with respect to each other, as was assumed in setting up our model.

In their experiments, Priestley and his co-workers also found effects which are most plausibly explained⁽⁶⁾ by joining the α and γ pockets as shown in Figure 22. There does not seem to be any other way of arranging the carrier

pockets to agree with all the DHVA data. This implies, however, that the bands under consideration have their energy extrema along the TW axis, where there is no inversion symmetry, and therefore there is no reason to expect that the extrema of the two bands should be coincident. It can be shown, however, (See Appendix A) that if there was any appreciable displacement of the band extrema with respect to each other, the relative amplitudes of the n_t -even and the n_t -odd oscillations should be complicated oscillatory functions of field. Our experimental data show no traces of any such behavior, and upon estimating the maximum displacement of the band extrema which could have gone unnoticed in our experiments, we find that this displacement must be equal to or smaller than the very small displacement* shown in Figure 23b.

Because of the good agreement between the cyclotron effective mass measured for the trigonal magnetorefectivity oscillations, and the corresponding mass measured for the γ carriers,⁽⁶⁾ we are inclined to continue to associate these magnetorefectivity oscillations with transitions involving this band, and assume that the near coincidence of the band extrema is due to relations between the bands which are not yet completely understood. This situation would not be unprecedented. In bismuth, for example, we have experimentally found relations between the bands near the Fermi surface at the L point in the Brillouin zone, which are not predicted by any simple symmetry argument, though these relations can be understood in terms of the complicated argument advanced by Abrikosov.⁽¹³⁾ (For details, see Section IIC.)

* The extremum-to-extremum displacement is less than, or equal to .0052 atomic units, while the distance between the T and W points is .476 atomic units.

Although we cannot completely understand the reason for the near coincidence of the band extrema in As, the band model of Lin and Falicov⁽¹⁾ does give us some very good clues as to the cause. To discuss this point, we will first refer back to Figure 23, where we show the theoretical band structure along the TW or binary axis. (See Section IA for discussion.) In part a of this figure, we display the bands as calculated by Lin and Falicov, neglecting spin orbit coupling. The accidental cross-over degeneracy would be split by spin orbit coupling, giving rise to the γ carrier band and the nearby strongly coupled band,⁽¹²⁾ as is shown in detail in Figure 23b. This alone would indicate that the two band extrema should lie close to each other. Furthermore, the calculated bands of Figure 23a have very nearly equal and opposite slopes at the crossover degeneracy which also indicates that the band extrema of Figure 23b should be very nearly coincident.

The assumption that the small band gap under consideration is due to spin orbit coupling is also consistent with our data. The spin orbit splitting at the T point for arsenic was estimated to be .24-.32 eV by Falicov and Golin,⁽⁶⁷⁾ which makes it reasonable to find a spin-orbit splitting of .172 eV at a point a small distance from T. We therefore conclude that the results of the magneto-reflection experiments with the magnetic field parallel to the trigonal axis are consistent with the results of the Lin-Falicov⁽¹²⁾ band model for arsenic, even though this band model seems to be in error at the nearby T point.

We have now justified all of the assumptions we made in setting up our band model back at the beginning of this section, with the exception of the assumption that the effects of spin-orbit coupling on the Landau levels can be ignored. In order to show that this is true, in spite of the fact that the gap itself is produced by spin-orbit coupling, we refer back to the work we did on

bismuth. (See Section IIID). First we note that the two band model of Lax can treat spin-orbit coupling of arbitrary strength,⁽³⁵⁾ and is applicable at $k_z = 0$ in arsenic, where we have, essentially, two coincident strongly interacting bands. Furthermore, we note that the Lax model predicts that the eigenfunctions and Landau level spin splittings for the two bands will be related to each other.⁽¹⁰⁾ In particular, in the region where the parabolic approximation holds ($\hbar\omega_c \ll E_g$), we find that we can relabel the spin states so that the selection rule for the strong transitions is $\Delta S = 0$ with equal g^* factors for the two bands. We would also expect that these selection rules and g^* factors would continue to apply even when $k_z \neq 0$, as long as the energy bands were still essentially parabolic, so that the only changes that the spin-orbit effects would produce in the conductivity are the unobservable ones associated with the Fermi level cutoff.

In summary, we feel that there is available an adequate model to explain the available data on the oscillations in the magnetorefectivity of arsenic in the trigonal sample orientation. In the next section, however, we will suggest some future experiments that could shed more light on the properties of this material.

SECTION IVE

SUMMARY

First of all, we have observed a series of oscillations in the magneto-reflectivity due to interband transitions with a critical point at T in the Brillouin zone, and an energy gap of .346 eV. Furthermore, from the fact that these oscillations are extinguished when the optical electric field is perpendicular to the trigonal axis, we have obtained some information about the possible symmetry types of the bands involved in the transition. Upon comparing these results with the pseudopotential calculation of Lin and Falicov,⁽¹²⁾ however, it is found that Lin and Falicov do not predict a small band gap at T for bands of these symmetry types. This indicates that some additional theoretical work is required.

We have also observed a Fermi level cutoff in this series of oscillations, which seems to indicate that there are carriers associated with one of the bands. We estimate that the number of carriers involved is very small, but perhaps their properties could be explored using some of the very sensitive modern DHVA techniques. An attempt to do this should certainly be made.

Secondly, we have observed some very large oscillations in the magneto-reflectivity when H is parallel to the trigonal axis, which are interpreted as being due to interband transitions with an energy gap of .172 eV. Furthermore, our data seem to be consistent with assuming that these transitions are between the bands which give rise to the γ necks in the band model of Lin and Falicov.⁽¹²⁾ To test this hypothesis out in more detail, however, it would be very interesting to study the oscillations in the magnetorefectivity when the magnetic field is not along one of the principal crystalline axes, and to

compare the observed angular dependence with the very striking angular dependence we would expect if our explanation were correct. This could be done by either:

a) using the Faraday geometry and a sample with an optical face cut at an angle to the principal axes; or

b) using the Voigt geometry, where we can vary the direction of the magnetic field merely by rotating the sample.

APPENDIX A

CONDUCTIVITY OF THE ARSENIC TRIGONAL FACE

In this appendix, we will consider the oscillations in the magnetoreflexivity produced by direct interband transitions between Landau levels associated with two non-degenerate parabolic bands with energy extrema lying along the TW axes, which are axes of two-fold rotation in the Brillouin zone of arsenic. We will use the usual notation for the coordinate axis system, with the x-axis the axis of two-fold rotation, the z-axis the trigonal axis, and the y-axis the third member of the orthogonal set. We will further restrict ourselves to the case where the two bands interact very strongly in the x and y directions, and very weakly in the z-direction, and where both the magnetic field and the propagation vector of the light are parallel to the trigonal axis. For simplicity, the effects of spin will be ignored.

Since we have restricted ourselves to parabolic bands, we may write ψ_j , the wave function for band j, as

$$\psi_j = F_j U_j, \quad (\text{AA1})$$

where F_j is the envelope function and U_j is the core wave function at $\vec{K}_0$, the point in the Brillouin zone from which we will measure the crystalline momentum. Since there is no inversion symmetry for a general point⁽⁶⁷⁾ along a two-fold axis, the extrema of the two bands need not be coincident, so we will define $\vec{K}_0$ as the point on the two-fold axis midway between the energy band extrema.

The envelope function is found by solving the single band, spinless effective mass secular equation⁽⁶¹⁾ for band j

$$\{E_j^0 + (\vec{\pi} + \hbar \vec{a}_x D) \cdot \frac{\vec{\alpha}^j}{2m_0} \cdot (\vec{\pi} + \hbar \vec{a}_x D)\} F_j = E_j F_j \quad . \quad (\text{AA2})$$

where E_j^0 is the energy of band j at $\vec{K}_0$, D is one half the displacement between the band extrema, $\vec{a}_x$ is the unit vector in the x -direction, $\vec{\alpha}^j$ is the dimensionless reciprocal effective mass tensor for band j , and

$$\vec{\pi} = \vec{p} - \frac{e\vec{A}}{c} \quad . \quad (\text{AA3})$$

Due to the two-fold rotation about the x -axis

$$\alpha_{xy}^j = \alpha_{zx}^j = 0 \quad . \quad (\text{AA4})$$

Furthermore, because the two bands interact strongly in x and y directions

$$\alpha_{xx}^u = -\alpha_{xx}^l = \alpha_{xx} \quad , \quad (\text{AA5a})$$

and

$$\alpha_{yy}^u = -\alpha_{yy}^l = \alpha_{yy} \quad , \quad (\text{AA5b})$$

where $j = u, l$ for the upper and lower bands, respectively. The remaining components of the effective mass tensors are unrelated, so that one expects the constant energy surfaces for the two bands to be tilted with respect to each other in the y - z plane.

Choosing the gauge where $\vec{A}$ is parallel to the y -axis, and solving Eq. AA2, we find

$$F_j = e^{(izk_z + iyk_y + iDx)} \phi_n(x - x_j^0) \quad , \quad (\text{AA6})$$

where $\phi_n(x-x_j^0)$ is the harmonic oscillator function of index n centered at x_j^0 , where

$$x_j^0 = \lambda^2 \left[k_y + \frac{\alpha_{yz}^j}{\alpha_{yy}^j} k_z \right], \quad (\text{AA7a})$$

and λ is the characteristic length

$$\lambda = \sqrt{\frac{\hbar c}{eH}}. \quad (\text{AA7b})$$

The corresponding energy, E_j is

$$E_j = E_j^0 + \frac{\beta_0 H}{m_{cj}^*} \left(n + \frac{1}{2} \right) + \frac{\hbar^2 k_z^2}{2m_0} \left(\alpha_{zz}^j - \frac{[\alpha_{zy}^j]^2}{\alpha_{yy}^j} \right), \quad (\text{AA8})$$

where m_{cj}^* is the signed cyclotron effective mass, of magnitude $m_c^* \equiv (\alpha_{xx} \alpha_{yy})^{-1/2}$ and positive sign for the upper band, and equal magnitude and opposite sign for the lower band, and

$$\beta_0 = \frac{|e|\hbar}{m_0 c}. \quad (\text{AA9})$$

We next would like to calculate the velocity matrix elements for inter-band transitions between these states. Rather than use the complicated theoretical apparatus we have developed in Chapter III, however, we will attack the problem in a much more straightforward way. First of all, we may make the approximation⁽⁹⁰⁾

$$\int_{-\infty}^{\infty} \psi_j^* \vec{v} \psi_j' dx = \int_{-\infty}^{\infty} F_j^*(x) F_j'(x) dx \int_{-\infty}^{\infty} U_j^*(X) \vec{v} U_j(X) dX \quad (\text{AA10})$$

which is true, provided that the magnetic energy is much less than the band gap, because $\vec{v}$ involves a differentiation, and U_j is a very rapidly varying periodic function of $\vec{r}$, while F_j varies quite slowly with $\vec{r}$. We can, therefore, immediately write

$$\langle \psi_j | \vec{v} | \psi_j' \rangle = \vec{v}_{jj'} \hat{I}(n, n', t, w) \quad , \quad (\text{AA11})$$

where

$$\vec{v}_{jj'} = \langle U_j | \vec{v} | U_j' \rangle \quad , \quad (\text{AA12})$$

and $\hat{I}(n, n', t, w)$, the overlap integral is

$$\hat{I}(n, n', t, w) = \int_{-\infty}^{\infty} e^{2iDx} \phi_n(x - x_u^0) \phi_n(x - x_l^0) dx \quad . \quad (\text{AA13})$$

The dimensionless parameter, t , describes the displacement of the band extrema along the x -direction in the Brillouin zone, and is given by the expression

$$t = D\lambda \left(\frac{\alpha_{yy}}{\alpha_{xx}} \right)^{1/4} \quad . \quad (\text{AA14})$$

The dimensionless parameter, w , describes the relative displacement of the conduction and valence band orbits along the y -direction in the Brillouin zone due to the relative tilt of the corresponding constant energy surfaces, and is given by the expression

$$w = \frac{1}{2\lambda} (x_l^0 - x_u^0) \left(\frac{\alpha_{yy}}{\alpha_{xx}} \right)^{1/4} = \xi \lambda k_z \quad , \quad (\text{AA15})$$

where

$$\xi = \frac{1}{2} \left(\frac{\alpha_{yy}}{\alpha_{xx}} \right)^{1/4} \frac{\alpha_{yz}^u + \alpha_{yz}^l}{\alpha_{yy}} \quad . \quad (\text{AA16})$$

The reason we introduce these dimensionless parameters is that we find it convenient to work with the normalized harmonic oscillator function, $\theta_n(v)$, of the dimensionless argument v , where $\theta_n(v)$ is the solution to the normalized harmonic oscillator equation⁽⁹¹⁾

$$\left[-\frac{\partial^2}{\partial v^2} + v^2 \right] \theta_n(v) = r \theta_n(v) \quad , \quad (\text{AA17})$$

with the eigenvalues

$$r = 2n+1 \quad , \quad (\text{AA18})$$

and

$$v = \left(\frac{\alpha_{xx}}{\alpha_{yy}} \right)^{1/4} \frac{x}{\lambda} \quad . \quad (\text{AA19})$$

To evaluate the overlap integral, which can be now re-written

$$\hat{I}(n, n', t, w) = \int_{-\infty}^{\infty} e^{2itv} \theta_n(v+w) \theta_n(v-w) dv \quad , \quad (\text{AA20})$$

we may make use of several well known relations.⁽⁹¹⁾ First of all, we write $\theta_n(v)$ in the form

$$\theta_n(v) = (\sqrt{\pi} 2^n n!)^{-1/2} e^{-v^2/2} H_n(v) \quad , \quad (\text{AA21})$$

where $H_n(v)$ is the n^{th} Hermite polynomial. Defining a new variable of integration

$$q = v - it \quad , \quad (\text{AA22a})$$

and a new overlap parameter

$$b = t + iw \quad , \quad (\text{AA22b})$$

we may re-write the integral

$$\hat{I}(n, n', b) = \int_{-\infty}^{\infty} e^{-q^2 - bb^*} \frac{H_n(q+ib) H_{n'}(q+ib^*)}{(\pi 2^{n+n'} n! n'!)^{1/2}} dq \quad , \quad (\text{AA23})$$

where we may integrate along the real axis rather than along the line in the complex plane $\text{Im}(q) = -t$ (See Eq. AA22a) because the integrand displays no singularities in the region enclosed by these two paths.⁽⁹²⁾ To evaluate this integral, we next note that the Hermite polynomial only contains terms up to the n^{th} power in v , so that we may use a Taylor series expansion to write the exact relation

$$H_n(q+ib) = \sum_{m=0}^n \frac{(ib)^m}{m!} \frac{d^m}{dq^m} H_n(q) \quad . \quad (\text{AA24})$$

Furthermore, it can be easily established that

$$\frac{d^m}{dq^m} H_n(q) = \frac{2^m n!}{(n-m)!} H_{n-m}(q) \quad , \quad (\text{AA25})$$

so that we may write

$$H_n(q+ib) = \sum_{m=0}^n \frac{(2ib)^m}{m!} \frac{n!}{(n-m)!} H_{n-m}(q) \quad . \quad (\text{AA26})$$

Finally, from the orthonormality of the $\Theta_n(q)$ functions, we may readily establish

$$\int_{-\infty}^{\infty} e^{-q^2} H_n(q) H_{n'}(q) dq = \sqrt{\pi} 2^n n! \delta_{nn'}, \quad (\text{AA27})$$

Using Eq. AA26 to expand the Hermite polynomials in Eq. AA23, and Eq. AA27 to do the resulting integrals, we find

$$\hat{I}(n, n', b) = e^{-bb^*} \sqrt{n!n'!} (i\sqrt{2} b)^{n-n'} \sum_{m=0}^n \frac{(-2bb^*)^m}{(n-n'+m)! (n'-m)! m!}, \quad (\text{AA28})$$

provided that $n \geq n'$. If this is not the case, we can always interchange n and n' and use Eq. AA28, only making an error in the phase of the integral. This phase, however, has no physical significance, so that we will, in fact, replace the complex quantity b by its magnitude B , and define the overlap integral function $I(n, n', B)$ as

$$I(n, n', B) = e^{-B^2} \sqrt{n!n'!} (\sqrt{2} B)^{n-n'} \sum_{m=0}^n \frac{(-2B^2)^m}{(n-n'+m)! (n'-m)! m!}. \quad (\text{AA29})$$

In order to explore the lineshape of the magnetorefectivity oscillations arising from the interband transitions between the Landau levels of the upper and lower bands, we would now like to calculate the conductivity at optical frequencies due to these transitions, using Eq. IIIA25. In particular, we are most interested in the conductivity in the x and y directions, since the light is propagating in the z -direction. Using the velocity matrix elements and Landau level energies we have found, we would then wish to calculate

$$\sigma_{jj} = \frac{e^2 \alpha_{jj} E_g}{2m_0 (\lambda \pi)^2} \sum_{n, n', M} \int_{k_a}^{k_b} \frac{dk_z I^2(n, n', B)}{\Delta E \left(\frac{iM}{\hbar} \Delta E - i\omega + 1/\tau \right)}, \quad (\text{AA30})$$

where we have defined:

$$B \equiv \sqrt{t^2 + w^2} = \lambda \sqrt{D^2 \left(\frac{\alpha_{yy}}{\alpha_{xx}} \right)^{1/2} + \xi^2 k_z^2} \quad ; \quad (\text{AA31a})$$

$$\Delta E \equiv E_g + \frac{\beta_o H}{m_c^*} (n+n'+1) + \gamma \frac{\hbar^2 k_z^2}{2m_o} \quad ; \quad (\text{AA31b})$$

$$\gamma \equiv \alpha_{zz}^u - \alpha_{zz}^l - \frac{(\alpha_{yz}^u)^2 + (\alpha_{yz}^l)^2}{\alpha_{yy}} \quad ; \quad (\text{AA31c})$$

$j = x$ or y ($\sigma_{xy} = 0$); E_g is the energy band gap; $M = +1, -1$, for upper to lower, and lower to upper band transitions, respectively; k_a and k_b are the limits of integration arising from the Fermi factors; ^{*} and we have replaced the portion of the velocity matrix element involving the core wave functions (See Eqs. AA11 and 12) with the value for this quantity obtained from the f-sum rule, assuming that all the curvature of the upper band in the x and y directions is produced by its interaction with the lower band, and visa versa.

Eq. AA30 describes the contribution to the conductivity from one critical point. It is also most useful to have an expression for the total contribution to the conductivity from all of the six critical points of this type. We will call this conductivity tensor σ^T , and expect that

$$\sigma_{xx}^T = \sigma_{yy}^T \equiv \sigma_{\perp} \quad (\text{AA32})$$

since the magnetic field is along the trigonal axis.

^{*}In order to simplify the integration, we only integrate in the range $k_z \geq 0$.

It may then be easily shown that

$$\sigma_{\perp} = 3(\sigma_{xx} + \sigma_{yy}) \quad , \quad (\text{AA33})$$

where σ_{xx} and σ_{yy} are given by Eq. AA30.

Unfortunately, evaluating Eq. AA30 would prove to be a very formidable task. The essential problem is that each of the integrals over k_z must be done numerically* and since we must sum over both n and n' , the problem would take much too much time. Let us therefore first consider the case where we have two bands whose energy extrema are displaced with respect to each other, but whose constant energy surfaces are both at the same angle, so that $\xi = 0$. In this case, $B = t$, which is not a function of k_z (See Eq. AA14) so that we may do all of the integrals analytically, with the intensity of the transition directly proportional to the overlap integral squared. Since $\theta_n(v)$ is an oscillatory function of v , however, the overlap integral is also an oscillatory function of t . Therefore, because t is proportional to $H^{-1/2}$, we conclude that if the main contribution to the amplitude of the n_t -odd oscillations comes from the relative displacement of the bands, the amplitudes of the oscillations would be oscillatory functions of field. In other words, if we measured the amplitude of an oscillation of fixed n_t as a function of field and photon energy, we would expect that in this case the amplitude of this oscillation would itself be an oscillatory function of field. Since no such effects are noted, we conclude that the main contribution to the amplitude of the n_t -odd oscillations comes from the relative tilt of the constant energy

* We have used a modification of what was called Method I in Appendix D.

surfaces of the bands. In this case, B is a function of k_z , and in integrating over k_z , we essentially average out the oscillations in $I(n, n', B)$.

Although we now know that D is small, it is probably not zero, so we desire a rough estimate of the maximum value it could have without giving rise to noticeable effects. To develop this estimate, we first note that the major contribution to the amplitude of the n_t -even oscillations comes from the $n = n'$ transition. In particular, even if $\xi \neq 0$, the amplitude of this oscillation is essentially proportional to $I^2(n, n, t)$, due to the peak in the joint density of states when k_z , and therefore w , are equal to zero. Therefore, when t becomes large enough (i.e. H becomes small enough) so that $I(n, n, t)$ goes through its first zero, the amplitude of the $n_t = 2n$ oscillation should be very strongly affected. We may follow the $n_t = 2$ oscillation down to 20 kG with a high enough signal to noise ratio so that we can be sure no such effect occurs. Therefore, we can be sure that at this value of field, t is still small enough so that $I(1, 1, t)$ has not yet gone through its first zero. From our calculation of $I(1, 1, t)$ we find that the first zero occurs at $t = .71$, so from Eq. AA14 we conclude that D must be smaller than .0026 atomic units* to keep t smaller than .71 at a value of λ corresponding to a field of 20 kG. For α_{xx} and α_{yy} , we have used the values in Table III derived from the data of Priestley. Figure 23 is drawn with this maximum permissible value for D .

Due to the smallness of the value of D , we see that we must consider, in detail, the case where $\xi \neq 0$ in order to explain the oscillations in the

* one atomic unit = (one hydrogen atom radius)⁻¹ or $1.89 \times 10^8 \text{ cm}^{-1}$.

magnetorefectivity which we have observed. For simplicity, we will therefore set $D = 0$. It will also prove convenient to calculate ϵ , the effective dielectric constant, where

$$\epsilon = \frac{4\pi\sigma_{\perp}}{-i\omega}, \quad (\text{AA34})$$

rather than $\sigma_{\perp}$, since it is most natural to discuss the optical properties of a material in terms of ϵ . It is also quite convenient to regroup the summations in Eq. AA30 over n and n' , and write

$$\epsilon = \sum_{M=-1}^{+1} \sum_{n_t=0}^{\infty} \epsilon(n_t, M), \quad (\text{AA35})$$

where

$$\epsilon(n_t, M) = \frac{6e^2 E_g (\alpha_{xx} + \alpha_{yy})}{\pi\omega\lambda^2 m_0} \sum_{n=0}^{n=n_t} \int_{k_a}^{k_b} \frac{dk_z I^2(n, n_t - n, \xi\lambda k_z)}{\Delta E \left[\frac{M}{\hbar} \Delta E - (\omega + i/\tau) \right]}. \quad (\text{AA36})$$

Therefore, $\epsilon(n_t, 1)$ represents the contribution to ϵ from all the transitions with the resonance at the same critical field, and $\epsilon(n_t, -1)$ is the corresponding non-resonant contribution.

We must now choose the parameters we will use in calculating $\epsilon(n_t, 1)$, the portion of ϵ of greatest interest. From our experiment, we set $E_g = .175$ eV, and $m_c^* = .031$. Since m_c^* is a function of energy, these numbers represent average values that describe our data in the region of interest. From the measurements of Priestley,⁽⁶⁾ we can derive the ratios between the elements of the α tensor, and upon requiring m_c^* to be .031, we find:

$$\alpha_{xx}^l = -\alpha_{xx} = -20.79 \quad , \quad (\text{AA37a})$$

$$\alpha_{yy}^l = -\alpha_{yy} = -51.85 \quad , \quad (\text{AA37b})$$

$$\alpha_{zy}^l = -8.998 \quad , \quad (\text{AA37c})$$

and

$$\alpha_{zz}^l = -1.059 \quad . \quad (\text{AA37d})$$

In order to find k_a and k_b , we calculate γ_l , where we define

$$\gamma_l \equiv \alpha_{zz}^l - \frac{(\alpha_{yz}^l)^2}{\alpha_{yy}^l} \quad , \quad (\text{AA38})$$

so that

$$E_l = -\frac{\beta_o H}{m_c^*} (n+1/2) + \gamma_l \frac{\hbar^2 k_z^2}{2m_o} \quad , \quad (\text{AA39})$$

where $E_l = 0$ at the extremum of the lower band. We find that $\gamma_l = +.502$, so that the sign of γ_l is positive, as would be expected from the fact that the γ carrier Fermi surface is a flared cylinder. Therefore, $k_a = 0$, and

$$\hbar k_b = \sqrt{2m_o \frac{([n + \frac{1}{2}] \beta_o H / m_c^* + E_f)}{\gamma_l}} \quad , \quad (\text{AA40})$$

where $E_f = -.01$ eV. We also may define

$$\xi_l \equiv \frac{\alpha_{yz}^l}{2\alpha_{yy}^l} \left(\frac{\alpha_{yy}^l}{\alpha_{xx}^l} \right)^{1/4} \quad , \quad (\text{AA41})$$

in which case, we find $\xi_l = .109$. We do not have any experimental evidence to determine the corresponding quantities, ξ_u and γ_u for the upper band, so we have assumed that ξ_u is about zero, and γ_u is about one, so that $\xi = .1$ and $\gamma = .5$. Finally, we must choose a value for τ . It is found that setting $\frac{\hbar}{\tau} = .005$ eV gives oscillations of about the right sharpness. Furthermore, it is found that the large oscillations we have been discussing may still be seen, reduced in amplitude by a factor of only about one-third, at liquid nitrogen temperatures. Since such a temperature corresponds to an energy of about .006 eV, this temperature dependence indicates that we have chosen a reasonable value for τ .

Using these parameters, we have calculated $\epsilon(n_t, 1)$ for several different values of n_t , and displayed the real part in Figure 36 for a photon energy of .22 eV. Assuming that the amplitudes of the oscillations in the reflectivity are proportional to the amplitudes of the oscillations in the real part of the dielectric constant, as was discussed in Section IVD, we can find many points of agreement between the characteristics of the oscillations of Figure 36, and the oscillations which we have experimentally observed. In particular:

a) the amplitudes of the oscillations in $\epsilon(n_t, 1)$ are easily large enough to explain the amplitudes of the observed magnetorefectivity oscillations for photon energies near the plasma frequency;

b) the ratios between the amplitudes of the oscillations in Figure 36 are in approximate agreement with the data;

c) the amplitude of the n_t -even oscillations decrease with increasing n_t at a much greater rate than does the amplitude of the n_t -odd oscillations, as is experimentally observed; and

d) the ratios between the amplitudes of the oscillations in Figure 36 are found to be dependent upon their quantum numbers, n_t , but independent of photon energy, as is required to explain the data. It was, in fact, the inability of simpler band models to explain this peculiar feature of our experimental traces which lead us to explore the complicated one we have just presented.

The only large discrepancy between the measured and calculated oscillation amplitudes occurs for the $n_t = 6$ peak, which is experimentally found to be anomalously small. One way of decreasing this discrepancy would be to assume that D were non-zero, but small, which would increase the size of the n_t -odd oscillations and decrease the size of the n_t -even oscillations, the magnitude of the change increasing with increasing n_t . Our computer program had been originally written only to handle the $D = 0$ case, however, and we did not feel that a thorough exploration of this point was worth the trouble of re-programming.

We did, however, consider some band parameters other than the ones discussed in connection with Figure 36. In particular, we considered the possibility that the interaction of the two bands in the z -direction might be weak enough to allow γ to be a negative quantity. It was found, however, that when this happens, the critical field corresponds to a sharp minimum in the real part of the dielectric constant. Therefore we would call the sharp minimum between the $n_t = 1$ and $n_t = 2$ peaks, the $n_t = 0$ minimum, and label the remaining minima accordingly. Upon plotting the inverse resonance fields defined at these minima as a function of n_t , we would obtain an n_t intercept of about -2.5 , which does not agree with the theory at all. We therefore conclude that γ must be positive, as was assumed.

In closing, we should emphasize that the curves of Figure 36 were displayed mainly to show the general features of the oscillations predicted by our simple band model. We have not, however, made any attempt at obtaining a detailed fit to the data, since we have found that it is impossible to obtain a reasonable fit by summing over a small^{*} set of $\epsilon(n_c, M)$ contributions. Furthermore, as our work on bismuth clearly demonstrates, it is necessary to have a very good band model before one can obtain a reasonable fit to the data, so that even if we developed a suitable approximation technique which would allow us to do the sum out to large enough n_c , we might very well find that our job had only begun.^{**} There does, however, seem to be enough agreement between the general features of the theoretical and experimental oscillations for us to believe that the band model we have proposed is correct in its essential features.

* It takes about three hours to generate a reasonably detailed curve on an SDS 390 Computer, summing on n_c only up to $n_c = 10$.

** For example, it is quite possible that the nonparabolic effects would have to be included.

APPENDIX B

DETAILS OF THE NUMERICAL ANALYSIS

In this appendix, we will discuss our method of doing the integral over j of Eq. AD33b, and also will go into some of the associated problems of error control. (See Appendix D.) For convenience we will call the integral over j of Eq. AD33b, $S(D)$, where

$$S(D) = S(j_a, D) - S(j_b + 1, D) \quad , \quad (AB1)$$

with $S(j_\ell, D)$ defined as

$$S(j_\ell, D) \equiv \int_{j_\ell - \frac{1}{2}}^{j_o} \frac{K_u}{K_d} dK_3 I(D, 2j, K_3) \quad . \quad (AB2)$$

The quantity j_o is defined in Eq. AD32. It is quite easy to find $S(j_b + 1, D)$ by numerical integration (by Simpson's rule, for example) since for $j_o \leq j \leq j_b + 1/2$, the integrand is a smooth function of j since $K_d = 0$ in this region. Finding $S(j_a, D)$ is decidedly more difficult, however, for in the region where $j_o \geq j \geq j_a - 1/2$, we see (from Eqs. AD19a, 20, and 32) that the lower limit on the K_3 integral, namely K_d , is

$$K_d = \sqrt{2b_3(j_o - j)} \quad , \quad (AB3)$$

which is a very rapidly varying function of j near j_o .

Let us, however, consider the function, $\phi(j, D)$, where

$$\phi(j, D) = \int_{K_d}^{K_u} dK_3 I(D, 2j, K_3) + \int_o^{K_d} dK_3 I_o(D, 2j, K_3) \quad , \quad (AB4)$$

where we define

$$I_o(D, 2j, K_3) \equiv \frac{\frac{2K_3^2}{\hat{\epsilon}_o(\hat{\epsilon}_o^2 - \epsilon^2)} \left(1 - \frac{D\epsilon^2 b_3}{\hat{\epsilon}_o(\hat{\epsilon}_o^2 - \epsilon^2)} \right)}{-i\omega + \frac{1}{\tau} + 2iMD\hat{\epsilon}_o/h}, \quad (AB5)$$

and, using the notation of Eq. AD13 define

$$\hat{\epsilon}_o \equiv \hat{\epsilon}(2j_o, 0) \quad (AB6)$$

Upon comparing the functions $I_o(D, 2j, K_3)$ and $I(D, 2j, K_3)$, defined by Eqs. AB5 and AD16C, respectively, we see that they have precisely the same value at $j = j_o$ and $K_3 = 0$, and very similar values nearby. Therefore, one would expect $\phi(j, D)$ not to be a rapidly varying function of j near j_o , because one would expect that the singularity at j_o due to the rapid variation of K_d in the first integral of Eq. AB4 would be nearly cancelled out by the corresponding singularity in the second integral. Upon working these expressions out numerically, this is indeed found to be the case.

Since the integrals of $I_o(D, 2j, K_3)$ over both j and K_3 may be evaluated analytically, and we may integrate the smooth function, $\phi(j, D)$, by Simpson's rule, (76) we may now write

$$\begin{aligned} S(j_a, D) &= \sum_{r=0}^{r_n+1} C[r] \phi(r\Delta j, D) - \int_{j_a-1/2}^{j_o} dj \int_0^{K_d} dK_3 I_o(D, 2j, K_3) \\ &= \sum_{r=0}^{r_n+1} C[r] \phi(r\Delta j, D) \\ &\quad - \frac{\frac{4(2b_3)^{3/2} (j_o - j_a + 1/2)^{5/2}}{15\hat{\epsilon}_o(\hat{\epsilon}_o^2 - \epsilon^2)} \left(1 - \frac{D\epsilon^2 b_3}{\hat{\epsilon}_o(\hat{\epsilon}_o^2 - \epsilon^2)} \right)}{-i\omega + \frac{1}{\tau} + 2iMD\hat{\epsilon}_o/h}, \end{aligned} \quad (AB7a)$$

where

$$\Delta j = (j_0 - j_a + 1/2) / r_n, \quad (\text{AB7b})$$

and $C[r]$ are the Simpson's rule coefficients

$$C[r] = \begin{cases} \frac{1}{3} \Delta j, & r = 0 \text{ or } r_n + 1 \\ \frac{2}{3} \Delta j, & r \text{ even and } \neq 0, r_n + 1 \\ \frac{4}{3} \Delta j, & r \text{ odd} \end{cases} \quad (\text{AB7c})$$

The number of intervals, r_n is adjusted to give adequate accuracy. It is found that $\phi(j, D)$ is so smooth that $r_n = 2$ is sufficient, (error less than 1%).

We now must choose the quantities j_a and j_b such $j_a < j_0 < j_b$, with j_a and j_b far enough removed from the singularity at j_0 such that for $j \leq j_a$ and $j \geq j_b$ we may replace the sum of Eq. AD22 by an integral. Since our expressions are smooth functions of j when $j > j_0$, j_b is merely chosen to be the first integer greater than j_0 . To choose j_a , we use the same line of reasoning that we used to set up the accuracy parameter, t_s , where we were attempting to keep our region of integration away from the region in which $I(D, 2j, K_3)$ is a rapidly varying function of j . Since it is the rapid variation of K_d which is giving us the trouble near j_0 , by analogy with Eq. AD24 we choose j_a by requiring that K_d be much greater than the change in K_d when j changes by one, or

$$t_j K_d(j_a) = \frac{\partial K_d}{\partial j} = \frac{b_3}{K_d(j_a)}, \quad (\text{AB8})$$

where t_j is a number much less than one. Since, once again, it is the accuracy of the fourth order approximation technique of Eq. AD25 which determines our error, and since once again the constant of proportionality is less than one, the error, for a given choice of j_a , will be less than the corresponding value of t_j , raised to the fourth power. We, therefore, set $t_j = t_s = .3$ to keep our error less than 1%.

APPENDIX C

DETERMINING THE VECTORS $\vec{W}(j)$

In order to get numerical results for the conductivity, using the techniques of this thesis, we must find numerical values for the three, three-component vectors, $\vec{W}(j)$. There are many ways of doing this, since the conditions we have imposed on these vectors:

$$\alpha_{\gamma\beta} = \sum_j W_{\gamma}(j) W_{\beta}(j) \quad , \quad (\text{AC1})$$

$$\vec{W}(1) \times \vec{W}(3) \cdot \vec{H} = 0 \quad , \quad (\text{AC2a})$$

$$\vec{W}(2) \times \vec{W}(3) \cdot \vec{H} = 0 \quad , \quad (\text{AC2b})$$

and

$$\vec{W}(1) \times \vec{W}(2) \cdot \vec{H} < 0 \quad , \quad (\text{AC3})$$

do not uniquely determine them.

A convenient way of satisfying these conditions will now be presented. First, we will define an orthonormal set of vectors $\vec{h}$, $\vec{n}$, and $\vec{m}$, where: $\vec{h}$ is the unit vector parallel to $\vec{H}$; $\vec{n}$ is any convenient unit vector perpendicular to $\vec{H}$; and $\vec{m} = \vec{n} \times \vec{h}$. We may also assume that $\vec{W}(2)$ is perpendicular to $\vec{n}$. Finally, in order to satisfy Equation AC2, we require that $\vec{W}(3)$ be parallel to $\vec{H}$.

It is now relatively simple to determine $\vec{W}(1)$. First we may show

$$(\vec{n} \cdot \vec{\alpha} \cdot \vec{n})^{1/2} = \left(\sum_j [\vec{n} \cdot \vec{W}(j)]^2 \right)^{1/2} = |\vec{n} \cdot \vec{W}(1)| \quad , \quad (\text{AC4})$$

since

$$\vec{n} \cdot \vec{W}(2) = \vec{n} \cdot \vec{W}(3) = 0 \quad . \quad (\text{AC5})$$

We now know $\vec{n} \cdot \vec{W}(1)$ except for its sign. Using this information, we may find $\vec{m} \cdot \vec{W}(1)$ and $\vec{h} \cdot \vec{W}(1)$ to within the same sign, by employing the easily proven relationships

$$(\vec{m} \cdot \vec{\alpha} \cdot \vec{n}) / (\vec{n} \cdot \vec{W}(1)) = \vec{m} \cdot \vec{W}(1) \quad , \quad (\text{AC6a})$$

and

$$(\vec{h} \cdot \vec{\alpha} \cdot \vec{n}) / (\vec{n} \cdot \vec{W}(1)) = \vec{h} \cdot \vec{W}(1) \quad ; \quad (\text{AC6b})$$

so that we may now write

$$\vec{W}(1) = \pm (\vec{m} \cdot \vec{W}(1)) + \vec{n} \cdot \vec{W}(1) + \vec{h} \cdot \vec{W}(1) \quad , \quad (\text{AC7})$$

where all of the dot-products are known. We will pick the sign such that Eq. AC3 is true.

Next, to find $\vec{W}(2)$ we define $\vec{\alpha}^{(2)}$ by the relation

$$\alpha_{\beta\gamma}^{(2)} \equiv \alpha_{\beta\gamma} - W_{\beta}(1)W_{\gamma}(1) = W_{\beta}(2)W_{\gamma}(2) + W_{\beta}(3)W_{\gamma}(3) \quad , \quad (\text{AC8})$$

and then may proceed as we did for $\vec{W}(1)$, writing

$$(\vec{m} \cdot \vec{\alpha}^{(2)} \cdot \vec{m})^{1/2} = |\vec{m} \cdot \vec{W}(2)| \quad , \quad (\text{AC9a})$$

$$(\vec{h} \cdot \vec{\alpha}^{(2)} \cdot \vec{m}) / (\vec{m} \cdot \vec{W}(2)) = \vec{h} \cdot \vec{W}(2) \quad , \quad (\text{AC9b})$$

and

$$\vec{W}(2) = \vec{m} \cdot \vec{W}(2) + \vec{h} \cdot \vec{W}(2) \quad . \quad (\text{AC9c})$$

Finally, we may find $\vec{W}(3)$ in a similar manner, by first defining $\vec{\alpha}(3)$ as

$$\alpha_{\beta\gamma}^{(3)} \equiv \alpha_{\beta\gamma}^{(2)} - W_{\beta}(2)W_{\gamma}(2) = W_{\beta}(3)W_{\gamma}(3) \quad , \quad (\text{AC10a})$$

and then writing

$$\vec{W}(3) = \vec{h}(\vec{h} \cdot \vec{\alpha}(3) \cdot \vec{h})^{1/2} \quad . \quad (\text{AC10b})$$

Now that we have determined the three, three-component vectors $\vec{W}(j)$, we may calculate the contribution to the total conductivity tensor from each of the carrier pockets by combining the appropriate values of σ_{+-} , σ_{-+} and σ_{33} , with the corresponding values for $W_{\gamma}(j)$, using Eq. IIIC51.

APPENDIX D

LAX MODEL REFLECTIVITY CALCULATION

In Sections IIIC and D, we have derived some of the key formulas required to calculate the reflectivity as a function of magnetic field and photon energy. There are, however, many steps in the calculation which we have not yet discussed. First of all, we must work out the sums and integrals in Eqs. IIID77 and 80 by numerical means. The more straightforward ways of doing this turn out to be hopelessly time consuming, and a considerable amount of effort was required to generate a computer program that would run with adequate speed. We will briefly discuss the techniques we used in this appendix.

Secondly, we must consider the dependence of the Fermi level and the number of carriers upon the magnetic field. At 100 kG, for example, the electron density may increase by a factor of three over its zero field value. To calculate the required quantities, we use the method of Smith, Baraff, and Rowell,⁽³⁹⁾ which we will describe in Appendix E.

In Appendix C, we will present a convenient method for calculating the three vectors $\vec{W}(j)$, which relate the ordinary, real space conductivity tensor, $\vec{\sigma}$, to the more easily calculated quantities σ_{+-} , σ_{-+} and σ_{33} . (See Eq. IIIC51.) Finally, in Appendix F, we will explain how one may use the conductivity tensor we have calculated to find the reflectivity of bismuth as a function of magnetic field and photon energy.

Let us now consider the evaluation of Eqs. IIID77 and 80. If one attempted to work out these equations by: a) doing the integrals over K_3 by Simpson's rule; and then b) summing over all of the possible inter-Landau level transitions; it would take a period of time that would be measured in months

to calculate a single theoretical magnetorefectivity curve in enough detail and with enough accuracy so that a meaningful comparison with experiment could be made. Since it was expected that we would have to try many different values for $\hbar/\tau$, the relaxation energy, in order to fit the experimental curves, a faster technique was clearly required.

The basic problem with Simpson's rule is that our integrand is a rapidly varying function of K_3 , due to the rapid variation of the resonance denominator when

$$\hbar\omega = M(E_1 - E_2) \quad , \quad (\text{AD1})$$

and the rapid variation of the Fermi functions when either

$$E_1 = \hat{\epsilon}_f \quad , \quad (\text{AD2a})$$

or

$$E_2 = \hat{\epsilon}_f \quad , \quad (\text{AD2b})$$

where $\hat{\epsilon}_f$ is the Fermi energy. Therefore, we must take very small intervals in K_3 in order to get an accurate value for our integral.

To circumvent the difficulties associated with the Fermi energy, we will assume $T = 0^\circ\text{K}$, since at liquid helium temperatures $k_b T$ is negligibly small (less than 10^{-3} eV). Therefore $f_1 - f_2$ is either zero or ± 1 , so we may rewrite Eq. IIID77 in the form

$$\sigma_M^F = \frac{e^2 \epsilon^2}{2m_o} C_k \sum_{D_1, D_2, n} \int_{K_a}^{K_b} dK_3 \frac{g(K_3)}{-i\omega + \frac{1}{\tau} + iMG(K_3)} \quad , \quad (\text{AD3})$$

where D_1 and D_2 are the band indicies as defined in Section IIID, and K_a and

K_b restrict the integral to those values of K_3 for which $f_1 - f_2 \neq 0$. In Eq. AD3 we have defined

$$G(K_3) \equiv (E_1 - E_2)/h, \quad (AD4)$$

and

$$g(K_3) \equiv \frac{|E_1 - E_2| K_3^2}{E_1 E_2 (E_1 + \epsilon)(E_2 + \epsilon)}, \quad (AD5)$$

where the absolute value sign arises from our use of the fact that

$$\frac{f_1 - f_2}{E_1 - E_2} \leq 0. \quad (AD6)$$

We could also treat Eq. IIID80 in a similar manner. As a matter of fact all of the techniques which will be discussed in this appendix may be applied to either Eq. IIID77 and 80 with equal ease, so for brevity, we will only discuss the evaluation of Eq. IIID77 in explicit detail.

The integrand of Eq. AD3 is still a rapidly varying function in the vicinity of the resonance described by Eq. AD1. We note, however, that $G(K_3)$ and $g(K_3)$ are relatively slowly varying functions of K_3 and may be accurately represented by a piecewise linear approximation. To generate this approximation we divide the range between K_a and K_b into m_n intervals, with $m_n + 1$ interval endpoints, $K(m)$; and choose m_n and $K(m)$ such that for K_3 within each interval m , (i.e. $K(m) \leq K_3 \leq K(m+1)$) the function $g(K_3)$ is well approximated by the expression

$$g(K_3) = A_1(m) + A_2(m)K_3, \quad (AD7)$$

where

$$A_1(m) = \frac{g\{K(m)\}K(m+1) - g\{K(m+1)\}K(m)}{K(m+1) - K(m)}, \quad (AD8a)$$

and

$$A_2(m) = \frac{g\{K(m+1)\} - g\{K(m)\}}{K(m+1) - K(m)}. \quad (AD8b)$$

Similar relations would hold between $G(K_3)$ and the piecewise linear approximation coefficients $B_1(m)$ and $B_2(m)$.

We may now approximately evaluate the integral of Eq. AD3 by writing

$$\int_{K_a}^{K_b} \frac{g(K_3) dK_3}{-i\omega + \frac{1}{\tau} + iMG(K_3)} \approx \sum_{m=0}^{m_n} \int_{K(m)}^{K(m+1)} \frac{(A_1(m) + A_2(m)K_3) dK_3}{-i\omega + \frac{1}{\tau} + iM(B_1(m) + B_2(m)K_3)}, \quad (AD9)$$

since we may do the integrals on the right side of this equation analytically. When we do this we have analytically taken into account the rapid variation of the integrand due to the resonance denominator, thereby circumventing the difficulties associated with the resonance of Eq. AD1.

We must now find a method of calculating the interval endpoints, $K(m)$, such that $g(K_3)$ and $G(K_3)$ will be closely approximated by our piecewise linear functions with a minimum number of intervals. One cannot, however, get an optimum piecewise linear fit to two different functions with one set of interval endpoints, so it is not quite clear how to choose $K(m)$ in an optimal fashion. We have, therefore, simply experimented with a number of different plausible techniques, until we found one which did our integrals with adequate speed and accuracy.

To calculate $K(m+1)$, given $K(m)$, we finally chose the recursion relation

$$\begin{aligned}
 K(m+1) - K(m) &= 2\sqrt{\epsilon} \left\{ \Lambda \frac{\partial^2 (|E_1| + |E_2|)}{\partial K_3^2} \bigg|_{K_3 = K(m)} \right\}^{-1} \\
 &= \frac{2}{\sqrt{\epsilon} \Lambda} \left\{ \frac{\epsilon^2 + \epsilon b_3 J_1}{|E_1(K(m))|^3} + \frac{\epsilon^2 + \epsilon b_3 J_2}{|E_2(K(m))|^3} \right\}^{-1}, \quad (AD10a)
 \end{aligned}$$

where Λ is the accuracy parameter. It works well because $g(K_3)$ and $G(K_3)$ both depend on E_1 and E_2 in such a way that their curvature is high when the curvature of $|E_1| + |E_2|$ is high, and low when the curvature of $|E_1| + |E_2|$ is low. Therefore the interval is small when the curvatures of $g(K_3)$ and $G(K_3)$ are large and we require high accuracy; on the other hand the interval is large when the curvatures of $G(K_3)$ and $g(K_3)$ are small so that we may achieve high speed. Since

$$\lim_{K_3 \rightarrow \infty} \frac{\partial (|E_1| + |E_2|)}{\partial K_3} = 2\sqrt{\epsilon}, \quad (AD10b)$$

we see that Λ , the accuracy parameter, is of the order of the number of intervals used. When $\Lambda = 40$, the technique we have been describing, which we call Method I, always makes an error of less than 1%. It is the most generally applicable of all the numerical integration techniques which we will discuss.

Although this technique is orders of magnitude faster than a Gaussian quadrature technique of comparable accuracy, the calculation would still take much too long if we used Method I exclusively. An even faster technique,

which we will call Method II, is applicable, however, whenever we are dealing with an interband transition for which $(E_1 - E_2)^2 \gg \epsilon b_3$.

To set up Method II, we will first introduce the quantity J , using the definition of Eq. IIIE9, so that we may write E_1 and E_2 in the simpler forms

$$E_1 = D \sqrt{\epsilon^2 + \epsilon b_3 J_1 + K_3^2 \epsilon} \quad (\text{AD11a})$$

and

$$E_2 = -D \sqrt{\epsilon^2 + \epsilon b_3 J_2 + K_3^2 \epsilon} \quad (\text{AD11b})$$

where we have set $D_1 = -D_2 \equiv D$ because we are considering an interband transition. We have set up the integrals of Eqs. IIID77 and 80 such that

$$J_1 = J_2 \equiv J$$

so that we may rewrite Eqs. AD11a and b as

$$E_1 = D \sqrt{\hat{\epsilon}^2 - \epsilon b_3} \quad (\text{AD12a})$$

and

$$E_2 = -D \sqrt{\hat{\epsilon}^2 + \epsilon b_3} \quad (\text{AD12b})$$

where $\hat{\epsilon}$ is given by

$$\hat{\epsilon}(J, K_3) = \sqrt{\epsilon^2 + \epsilon b_3 (J+1) + K_3^2 \epsilon} \quad (\text{AD13})$$

So far, no approximations have been made. Now, let us consider the approximations that may be made when $K_3 \gg K_2$, where K_2 is implicitly defined by the equation

$$t_b \{ (\hat{\epsilon}(J, K_3))^2 - \epsilon^2 \} = \epsilon b_3, \quad (AD14)$$

and t_b is a number much less than one. In that case, we may expand the square roots in Eq. AD12 to write

$$E_1 \approx D\hat{\epsilon} - D\epsilon b_3 / (2\hat{\epsilon}) \quad (AD15a)$$

and

$$E_2 \approx -D\hat{\epsilon} - D\epsilon b_3 / (2\hat{\epsilon}), \quad (AD15b)$$

where the fractional error in this approximation is always less than t_b^2 .

Furthermore, if we substitute Eqs. AD15a and b, into Eqs. AD4 and 5, we may show that

$$g(K_3) \approx \frac{2K_3^2}{\hat{\epsilon}(\hat{\epsilon}^2 - \epsilon^2)} \left(1 - \frac{D\epsilon^2 b_3}{\hat{\epsilon}(\hat{\epsilon}^2 - \epsilon^2)} \right), \quad (AD16a)$$

and

$$G(K_3) \approx 2D\hat{\epsilon}/h, \quad (AD16b)$$

with a fractional error always less than t_b^2 , so that if we define

$$I(D, J, K_3) \equiv \frac{\frac{2K_3^2}{\hat{\epsilon}(\hat{\epsilon}^2 - \epsilon^2)} \left(1 - \frac{D\epsilon^2 b_3}{\hat{\epsilon}(\hat{\epsilon}^2 - \epsilon^2)} \right)}{-i\omega + \frac{1}{\tau} + 2iMD\hat{\epsilon}/h}, \quad (AD16c)$$

then the fractional error between the integrand of Eq. AD3 and $I(D, J, K_3)$ will always be less than t_b^2 .

Therefore, one can approximately evaluate the integral of Eq. AD3 in the range $K_l \leq K_3 \leq K_b$ by using the expression

$$\int_{K_l}^{K_b} \frac{dK_3 g(K_3)}{-i\omega + \frac{1}{\tau} + iMG(K_3)} = \int_{K_l}^{K_b} dK_3 I(D, J, K_3) \quad , \quad (AD17)$$

since the integral on the right side may be done exactly by partial fractions. We therefore must use the slower technique of Method I only for intra-band transitions, and for interband transitions in the range $K_a \leq K_3 \leq K_l$. In our calculations, we have set $t_b = 0.1$ which gives us an error always less than 1%. The approach we have just described is Method II. It is still not fast enough, however, since for interband transitions, the sums in Eqs. IIID77 and 80 must be carried out to prohibitively large values of n . For example, if $\hat{\epsilon}_u = .2$ eV (the reasons for the choice of this value were explained in Section IIIF) and $\epsilon b_3 = 2.85 \times 10^{-5}$ eV² (which corresponds to a field of 10 kG parallel to the binary axis for the principal ellipsoid), then n_m , the upper limit for the sum over n , would be about 1,400 (See Eq. AD13.) To handle the interband transitions, therefore, it was necessary to develop Method III, in which we essentially replace the major portion of the sum over n by an integral which we can evaluate analytically. We do not run into similar difficulties for the intra-band transition, since in that case we need only consider the Landau levels which intersect the Fermi level, and they are few in number.

In order to discuss Method III, let us first make some convenient definitions. What we are essentially trying to evaluate here is $\xi(D)$, which we will define as the sum over n which appears in Eq. AD3;

$$\xi(D) \equiv \sum_{n=0}^n \int_{K_a}^{K_u} \frac{dK_3 g(K_3)}{-i\omega + \frac{1}{\tau} + iMG(K_3)} \quad (AD18)$$

In the sum above, we have set $D_1 = -D_2 \equiv D$ because we are restricting ourselves to interband transitions. Also for this reason, the upper limit of integration has become K_u , which is the value of K_3 beyond which our band model ceases to apply.

Let us now define

$$K_p^2 \equiv b_3(J+1) \quad (AD19a)$$

and

$$K^2 \equiv K_p^2 + K_3^2 \quad (AD19b)$$

so that

$$\hat{\epsilon} = \sqrt{\epsilon^2 + \epsilon K^2} \quad (AD19c)$$

In terms of these quantities, the portion of $\xi(D)$ which we will find convenient to evaluate by converting the sum to an integral will be that portion where $K^2 \geq K_o^2$. The choice of the quantity K_o^2 will shortly be discussed.

Once this quantity is chosen, however, we will use either Method I or Method II (whichever is applicable) only to integrate over the range $K_3 \leq K_d$, where we define

$$K_d \equiv \sqrt{K_o^2 - K_p^2} \quad (AD20)$$

It should be noted that K_d is a function of J .

The first requirement we place on K_0 is that

$$K_0^2 \geq b_3/t_b, \quad (AD21)$$

so that $K_d \geq K_l$ (See Eq. AD14) and we may use the approximations in Eqs. AD15 and 16 to simplify the expressions we must integrate. If $\xi_1(D)$ is that portion of $\xi(D)$ for which $K^2 \geq K_0^2$, we may now write

$$\xi_1(D) = \sum_{j=0}^{j_m} \int_{K_d}^{K_u} I(D, 2j, K_3) dK_3, \quad (AD22)$$

where $j \equiv J/2$ and j_m is a suitably defined upper limit. For K_u we will use the convenient expression

$$\epsilon K_u^2 = \hat{\epsilon}_u^2 - \epsilon^2 - \epsilon K_p^2. \quad (AD23)$$

The second restriction on K_0 stems from the requirement that the integrals over K_3 which appear in Eq. AD22 be smooth functions of the integer j , so that we may replace the sum over j with an integral. This requires that $\hbar\omega < 2\hat{\epsilon}$ so that $I(D, 2j, K_3)$ does not display resonant behavior. More specifically, we require that the fractional change in $2\hat{\epsilon} - \hbar\omega$ be very small when j changes by one, so that

$$t_s(2\hat{\epsilon}(J, K_d) - \hbar\omega) \geq \left. \frac{\partial(2\hat{\epsilon})}{\partial j} \right|_{K=K_0} = \frac{\partial \epsilon b_3}{\hat{\epsilon}(J, K_d)}, \quad (AD24)$$

where K_d is defined in Eq. AD20 and t_s is a number much smaller than one.

Once we have chosen K_0 to be the smallest value which satisfies both of the criteria we have just discussed, we may transform the sum over j in Eq. AD22 into an integral by using the well known formula⁽⁷⁴⁾

$$\sum_{j=j_1}^{j=j_2} f(j) \approx \int_{j_1-1/2}^{j_2+1/2} f(j) dj - \frac{1}{24} \left. \frac{df(j)}{dj} \right|_{j=j_1-1/2}^{j=j_2+1/2} \quad (AD25)$$

It can be shown that the approximation technique described by this formula is a fourth order process (the error is proportional to t_s^4) with a proportionality constant of less than one. We will therefore set $t_s = .3$ so that the final error of our approximation will be less than 1%.

Applying Eq. AD25 to Eq. AD22 we find

$$\begin{aligned} \xi_1(D) = & \int_{-1/2}^{j_m+1/2} dj \int_{K_d}^{K_u} dK_3 I(D, 2j, K_3) \\ & - \frac{1}{24} \frac{d}{d} \left\{ \int_{K_d}^{K_u} dK_3 I(D, 2j, K_3) \right\} \bigg|_{j=-1/2}^{j=j_m+1/2}, \end{aligned} \quad (AD26)$$

where we may conveniently determine j_m by requiring

$$\hat{\epsilon}_u^2 = \epsilon^2 + \epsilon b_3 (2(j_m+1/2)+1) \quad (AD27)$$

So far we have been careful to define the limits of integration: K_u , K_d , and $j_m+1/2$; such that the boundaries of the region of integration form circles in K_p, K_3 space. We may therefore easily do our integrals by first defining θ ,

$$\theta \equiv \arcsine(K_p/K) \quad (AD28a)$$

so that

$$K_3 = K \cos \theta \quad , \quad (AD28b)$$

and

$$K_p = K \sin \theta \quad ; \quad (AD28c)$$

in which case, it may be shown that

$$\begin{aligned} & \int_{-1/2}^{j_m+1/2} \int_{K_d}^{K_u} I(D, 2j, K_3) dK_3 dj \\ &= \frac{1}{b_3} \int_0^{K_{ou}} \int_{K_d}^{K_u} I(D, \frac{K_p^2}{b_3} - 1, K_3) dK_3 dK_p K_p \\ &= \frac{1}{b_3} \int_0^{K_{ou}} dK K^2 \int_0^\pi \sin \theta d\theta \cos^2 \theta \frac{\frac{K^2}{\hat{\epsilon}(\hat{\epsilon}^2 - \epsilon^2)} \left(1 - \frac{D\epsilon^2 b_3}{\hat{\epsilon}(\hat{\epsilon}^2 - \epsilon^2)} \right)}{-i\omega + \frac{1}{\tau} + 2iMD\hat{\epsilon}/\hbar} \quad , \end{aligned} \quad (AD29)$$

where

$$K_{ou} \equiv \sqrt{(\hat{\epsilon}_u^2 - \epsilon^2)/\epsilon} \quad . \quad (AD30)$$

The integrations over θ and K may both be done analytically.

In order to calculate $\xi(D)$, we must also evaluate the derivatives in Eq. AD26, and it turns out that the evaluation of the one associated with the lower limit offers some difficulty. Though the integrals we are to differentiate are analytical functions of j for negative j so long as

$$K_o^2 + b_3(2j+1) > 0 \quad , \quad (AD31)$$

the most convenient way of doing these integrals introduces a singularity just below $j = 0$. Since this singularity is spurious, and the integral itself is a smooth function of j near $j = 0$, we have approximated the derivative by its value at $j = 0$, where it can easily be found by numerical differentiation.

The procedure we have just described allows us to approximate the sum of Eq. AD22 by an integral which we may do exactly, but as it now stands, it still has a major flaw. In order to use Eq. AD25 we require that $f(j)$ be a smooth analytical function in the range $-1/2 \leq j \leq j_m + 1/2$, but the integral of Eq. AD22 is not such a function for j in the vicinity of j_0 , where j_0 is defined by the equation

$$K_0^2 = b_3(2j_0 + 1) \quad (\text{AD32})$$

At this value of j , the quantity K_d , the lower limit of the integral of Eq. AD22, has a singularity (See Eq. AD20), and the calculated conductivity will therefore display completely spurious DHS type oscillations as the Landau levels cross our nonphysical circle of radius K_0 in K_p, K_3 space.

To eliminate this difficulty, we actually perform the sum over j in the range $j_a \leq j \leq j_b$, where $j_a < j_0 < j_b$, and j_a and j_b are chosen far enough away from j_0 so as to avoid the difficulties associated with the singularity located at that point. This sum over j near j_0 will be called $\xi_2(D)$, where

$$\xi_2(D) = \sum_{j=j_a}^{j_b} \int_{K_d}^{K_u} dK_3 I(D, 2j, K_3) \quad (\text{AD33a})$$

when we add $\xi_2(D)$ to $\xi_1(D)$, we must of course also subtract the quantity $\xi_3(D)$, where

$$\begin{aligned}
\xi_3(D) &= \int_{j_a-1/2}^{j_b+1/2} dj \int_{K_d}^{K_u} dK_3 I(D, 2j, K_3) \\
&\quad - \frac{1}{24} \frac{d}{dj} \left\{ \int_{K_d}^{K_u} dK_3 I(D, 2j, K_3) \right\} \Bigg|_{j_a-1/2}^{j_b+1/2}
\end{aligned} \tag{AD33b}$$

corresponds to that portion of the integral of Eq. AD29 which is now being taken into account by the sum of $\xi_2(D)$.

This method of procedure introduces additional difficulties, however. First of all, the integral of Eq. AD33b cannot be done analytically, because the boundaries of the region of integration are not circles in K_p, K_3 space. Furthermore, in order to do this integral by a reasonably efficient numerical techniques, the singularity at j_0 must be handled in the proper way. These complications will be discussed in Appendix B, where we will describe the method that we used to do this integral. In this appendix, we will also discuss the method we used to pick j_a and j_b so that our calculation is both rapid and accurate. At this point, however, we will merely state that in obtaining the results displayed in Section IIIF we have chosen the various accuracy parameters such that the errors due to all the approximations made in calculating the conductivity are much less than 1%. This accuracy claim is substantiated by careful numerical comparison between the results of Methods I, II, and III. Method I was checked against a very detailed, and very slow, Simpson's rule integration.

Through the use of Method III, the computation time was finally brought down to a practical value. For example, to calculate the magnetorefectivity

curve of Figure 17 took about 2-1/2 hours on the SDS 930 computer we were using. It was felt that this speed would be adequate for our purposes, though it is amusing to note that a similar amount of data may be experimentally obtained in about 20 minutes.

APPENDIX E

THE FIELD DEPENDENT FERMI LEVEL

In a semimetal, the requirement of charge compenation determines the Fermi level.⁽³⁹⁾ Therefore, in a magnetic field, the Fermi level will always adjust itself so that the number of holes is equal to the number of electrons, and in bismuth, at high magnetic fields these shifts in the Fermi level can be quite appreciable.

To calculate the Fermi level, one must first be able to calculate N, the total density of carriers in a magnetic field for a single carrier pocket. This may be done by using the well known formula,⁽⁶⁹⁾ valid at T=0,

$$N = \frac{eH}{\pi\hbar c} \sum_{n,S} k_F(n,S) \quad , \quad (AE1)$$

where $\hbar k_F(n,S)$ is that value of the crystalline momentum parallel to the magnetic field at which the Landau level of orbital quantum number n, spin quantum number S, passes through the Fermi level. For the holes in bismuth, one may write for $\hbar k_F(n,S)$, using the results of Section IIIC⁽³⁹⁾

$$\hbar k_F^H(n,S) = \sqrt{2m_H [\hat{\epsilon}_{0,L} - \hat{\epsilon}_f - \hbar\beta^* (n + \frac{1}{2}) - \frac{e\hbar H}{4m_0 c} g^* S]} \quad , \quad (AE2)$$

where $\hat{\epsilon}_{0,L}$ is the displacement of the hole band edge from the zero of energy (set at the center of the band gap at L), g^* is the effective g factor for the holes, and m_H and β^* are to be calculated using the effective mass tensor for the hole band. For the electrons, we may write for $\hbar k_F(n,S)$, using the results of Section IIID⁽³⁹⁾

$$\hbar k_F^i(n, S) = \sqrt{m_H^i [\hat{\epsilon}_f^2 - \epsilon^2 - \epsilon b_3^i (2n+1-S)] / \epsilon} , \quad (\text{AE3})$$

where the i superscript labels the particular electron ellipsoid being considered.

Note that we have not included the splitting of the Lax degeneracy in this formula. The reason for this is that, at the fields at which the magneto-reflection oscillations may be observed, only the Landau level of lowest energy passes through the Fermi surface. Furthermore, as can be seen from Figure 14, the Lax model describes this Landau level very well in the vicinity of the Fermi energy.

In order to find the Fermi level, a computer program was written which adjusts $\hat{\epsilon}_f$ until the number of electrons is equal to the number of holes; that is, until

$$N^H = \sum_{i=1}^3 N^i . \quad (\text{AE4})$$

A calculated $\hat{\epsilon}_f$ vs. H curve for the Lax model is plotted in Figure 15. A very similar calculation was carried out by SBR (Smith, Baraff, and Rowell, ref. 39), who took into account the field dependence of the Fermi level in order to fit their DHS data. Their $\hat{\epsilon}_f$ vs. H curve is also shown in Figure 15 for comparison. It will be noted that their curve shows two peaks where our curve shows one. This is because they took into account the splitting of the Lax degeneracy, though in an incorrect manner. The energy displacement between the two curves is due to the fact that we have set our overlap energy, $\hat{\epsilon}_{0.L.}$, to that value which makes the number of carriers we calculate identical with the value measured by Smith, Baraff, and Rowell, and not to that value which makes the

zero field Fermi levels equal. The general features of the two curves are quite similar, however, which indicates that the gross dependence of the Fermi level on the magnetic field is insensitive to the splitting.

APPENDIX F

DETERMINING THE MAGNETOREFLECTIVITY

Once we have found the magnetic field and photon energy dependent total conductivity tensor $\overleftrightarrow{\sigma}$, where

$$\overleftrightarrow{\sigma} = \overleftrightarrow{\sigma}_{\text{electrons}} + \overleftrightarrow{\sigma}_{\text{holes}} - i\omega\overleftrightarrow{\epsilon}_{\text{core}}, \quad (\text{AF1})$$

we may proceed to calculate all of the electromagnetic properties of bismuth, including the infrared magnetorefectivity. These calculations are, however, considerably complicated by the anisotropic nature of our material. For example, in the presence of a magnetic field, the two characteristic modes of electromagnetic propagation will not, in general, be orthogonal to each other, and each mode will be elliptically polarized and have a non-zero longitudinal component of electric field.⁽⁶⁶⁾ The longitudinal components are particularly troublesome, since they lead to surface charge effects. Fortunately, we are most interested in the reflectivity for the binary face, and it may be shown, by simple symmetry arguments,⁽⁷⁵⁾ that when the magnetic field and the propagation vector of the light are parallel to either the trigonal or binary axes, the characteristic modes for electromagnetic propagation are purely transverse.

Let us work out the reflectivity for a linearly polarized beam of light propagating parallel to the binary axis, to illustrate how one may carry out these calculations.⁽⁶⁶⁾ First, we must find the two characteristic modes, $j = 1, 2$, with polarization vectors $\vec{a}(j)$, and corresponding effective conductivities, σ_j^{eff} . To do this, we must solve the secular equation

$$\begin{pmatrix} \sigma_{yy} & \sigma_{yz} \\ \sigma_{yz} & \sigma_{zz} \end{pmatrix} \begin{pmatrix} a_y(j) \\ a_z(j) \end{pmatrix} = \sigma_j^{\text{eff}} \begin{pmatrix} a_y(j) \\ a_z(j) \end{pmatrix}, \quad (\text{AF2})$$

where we have set $\vec{H}$ parallel to the binary axis, so that there are no simple relations between σ_{yy} , σ_{zz} , σ_{zy} , and σ_{yz} . Because the modes are purely transverse, $a_x(j) = 0$. In general, the polarization vectors for the two modes, $\vec{a}(1)$ and $\vec{a}(2)$ will be nonorthogonal and complex.

We next write the incident light beam as a linear combination of the two transverse modes. If the light were polarized parallel to the bisectrix (or y) axis for example

$$\vec{u}_y E_y = C_1 \vec{a}(1) + C_2 \vec{a}(2), \quad (\text{AF3})$$

where $\vec{u}_y$ is the unit vector parallel to the y axis, and C_1 and C_2 are two complex constants.

We next calculate r_j , the reflection coefficient at the air-material interface for mode j, using the standard formula⁽⁷⁷⁾

$$r_j = \frac{1 - \sqrt{\sigma_j^{\text{eff}} / (-i\omega)}}{1 + \sqrt{\sigma_j^{\text{eff}} / (-i\omega)}}. \quad (\text{AF4})$$

In general $r_1 \neq r_2$, so that the reflected electric field, $\vec{E}_r$, where

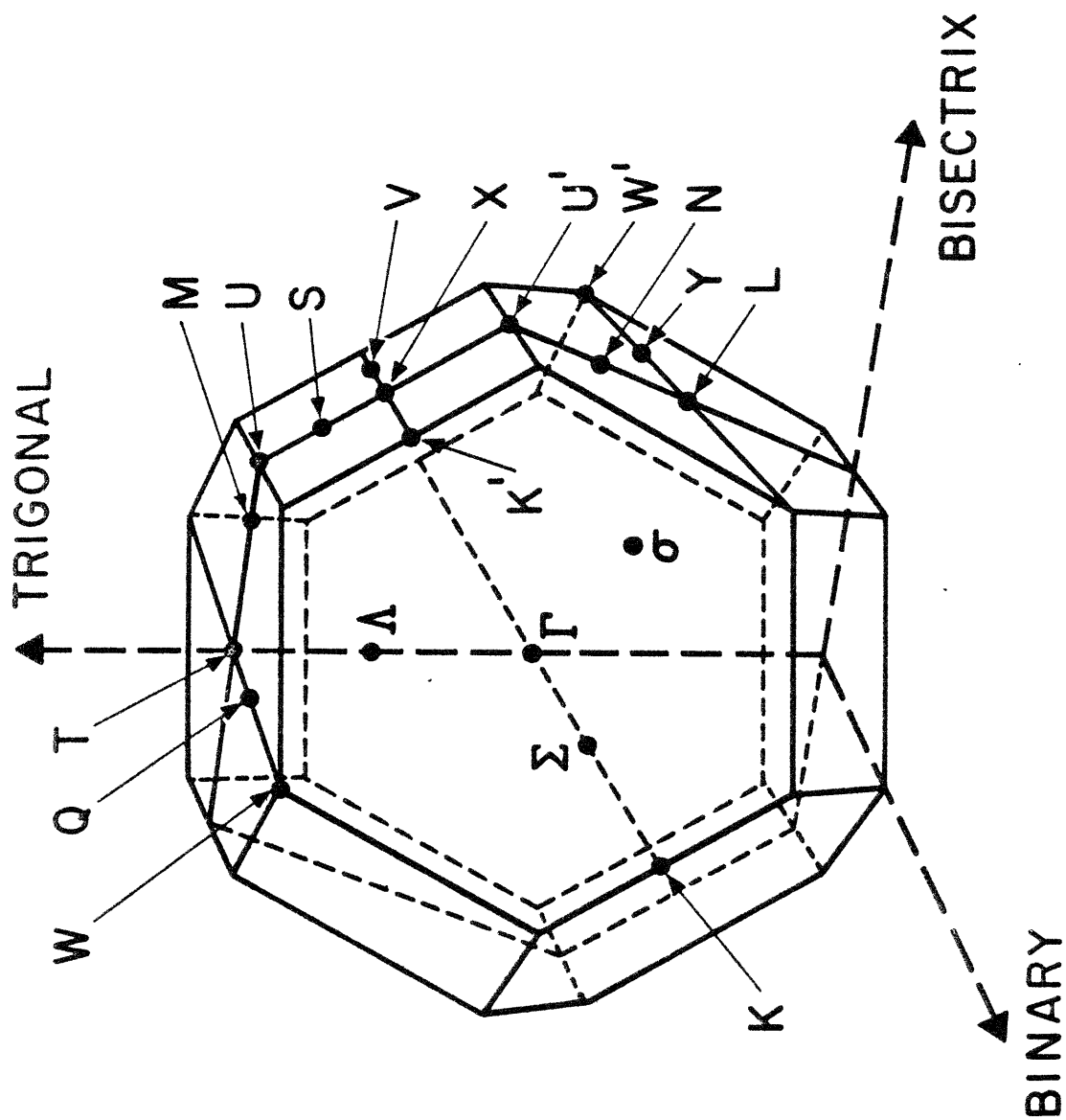
$$\vec{E}_r = C_1 r_1 \vec{a}(1) + C_2 r_2 \vec{a}(2), \quad (\text{AF5})$$

will no longer be linearly polarized along the y axis. Since, in our experimental system, there are essentially no polarizing components between the sample and the detector, the measured power reflectivity, R, will finally be the ratio of the total reflected power to the total incident power,

$$R = \frac{\vec{E}_r \cdot \vec{E}_r^*}{E_y^2} \quad (AF6)$$

BRILLOUIN ZONE FOR ARSENIC AND BISMUTH

FIGURE 1



MAGNETOREFLECTION EXPERIMENTAL SYSTEM

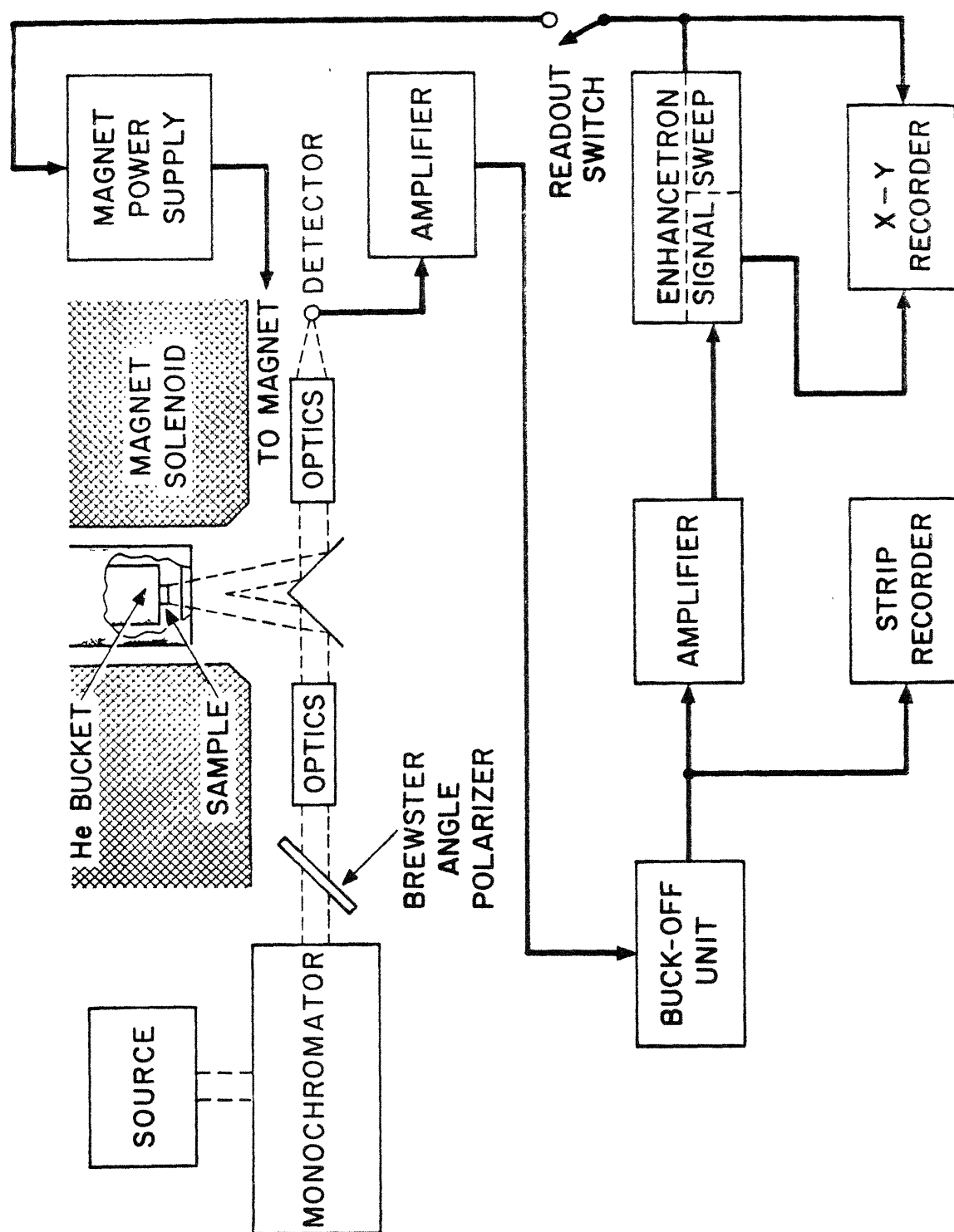


FIGURE 2

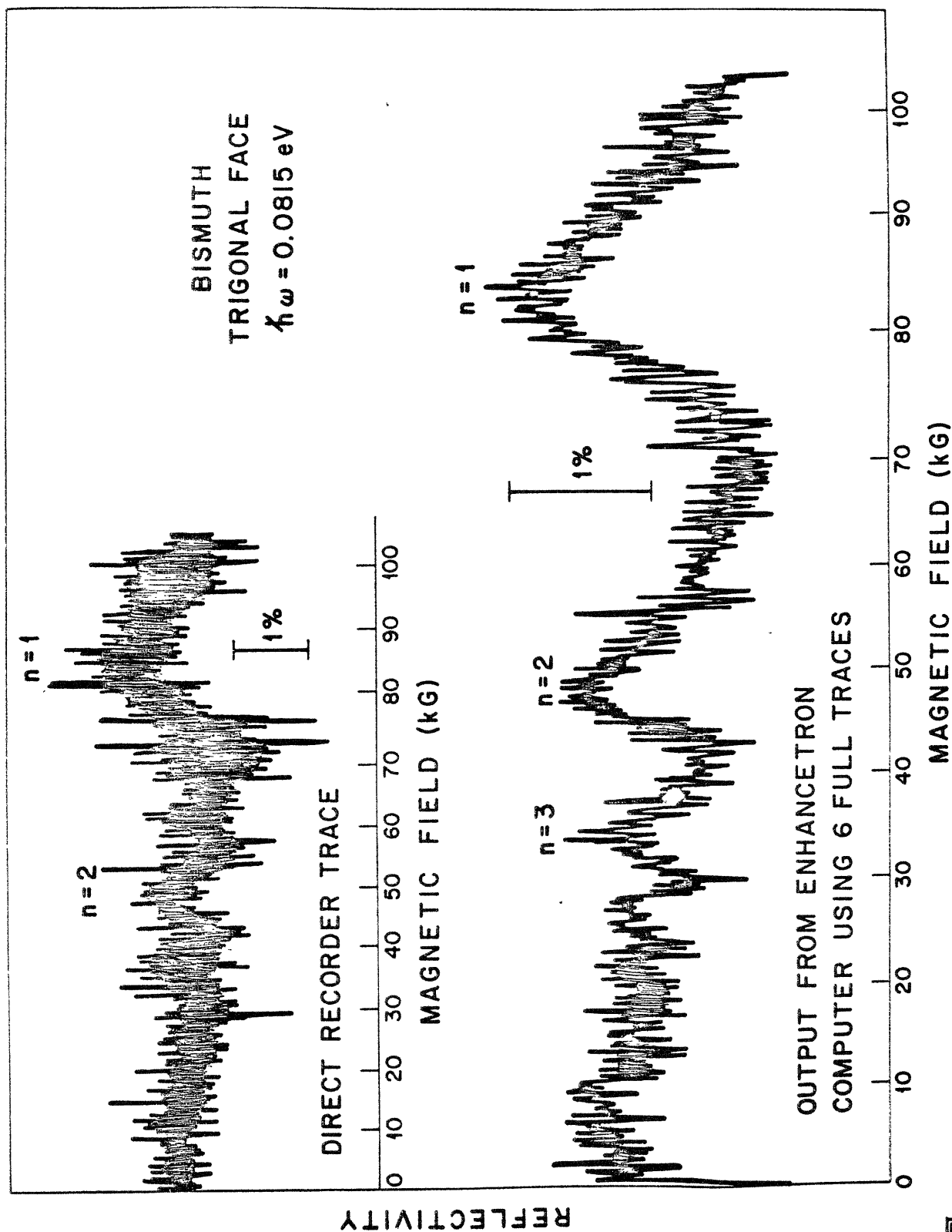


FIGURE 3

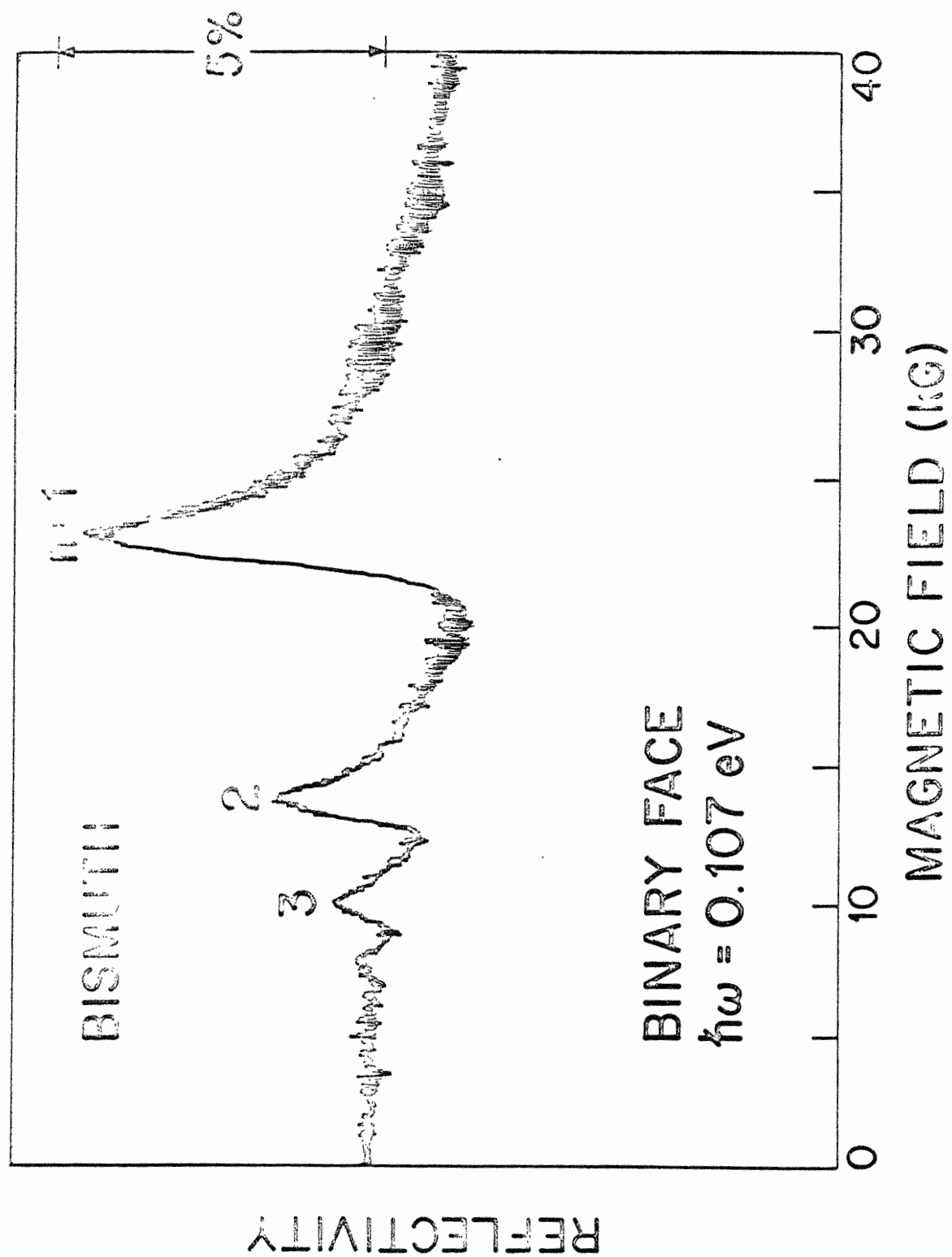
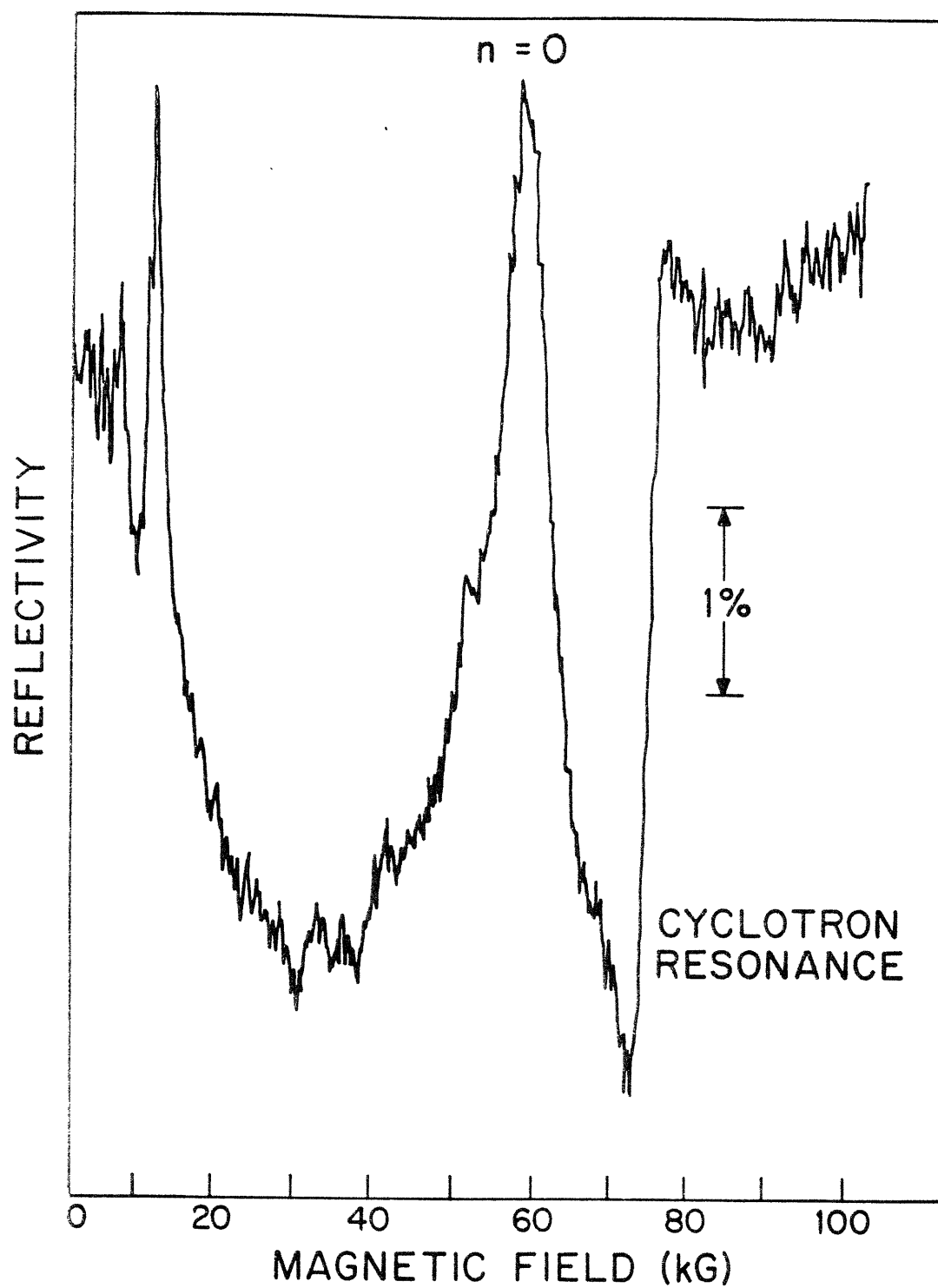


FIGURE 4



BISMUTH BINARY FACE
($\hbar\omega = 0.0751$ eV)

FIGURE 5

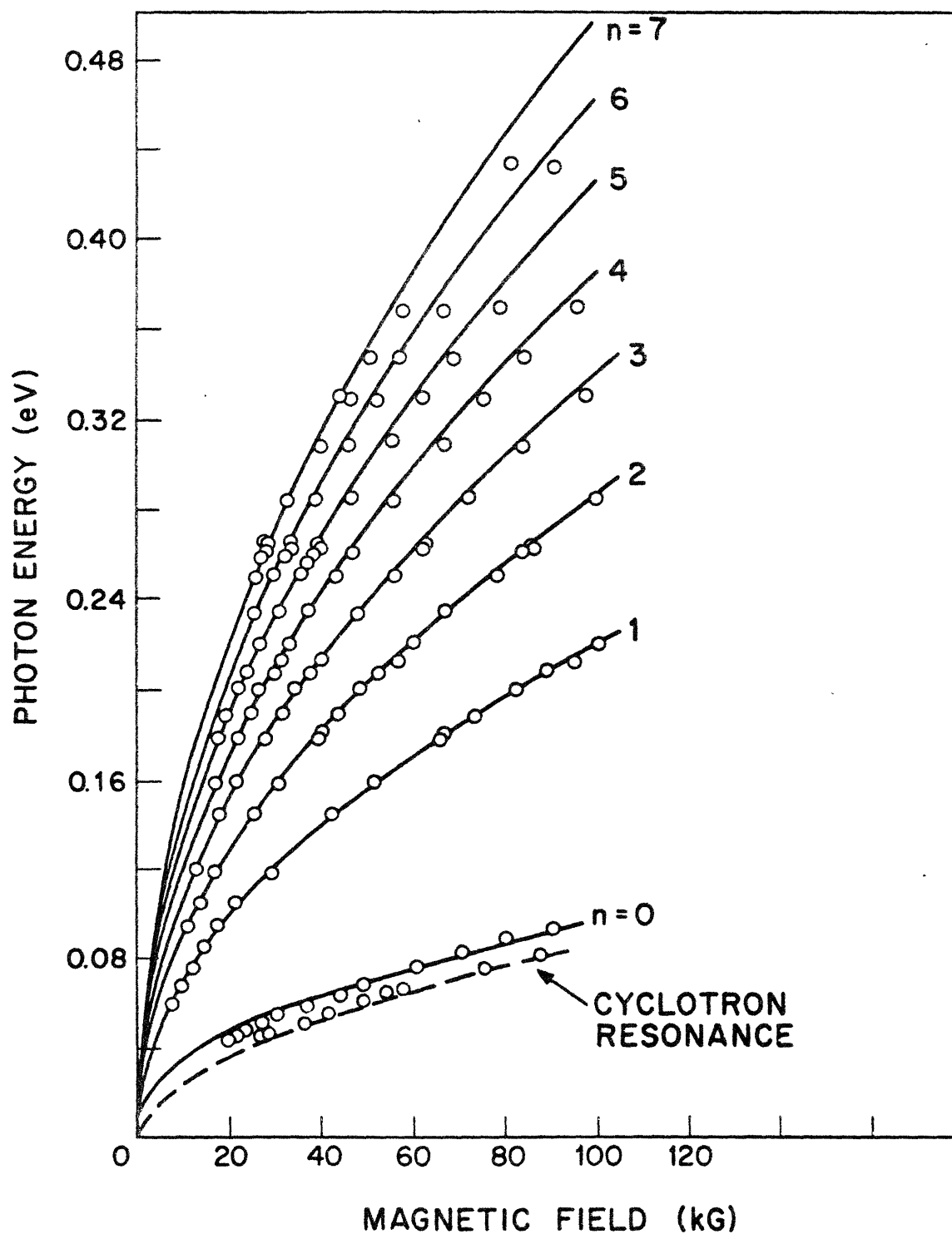


FIGURE 6

EXPERIMENTAL AND THEORETICAL RESONANCES
BISMUTH BINARY FACE

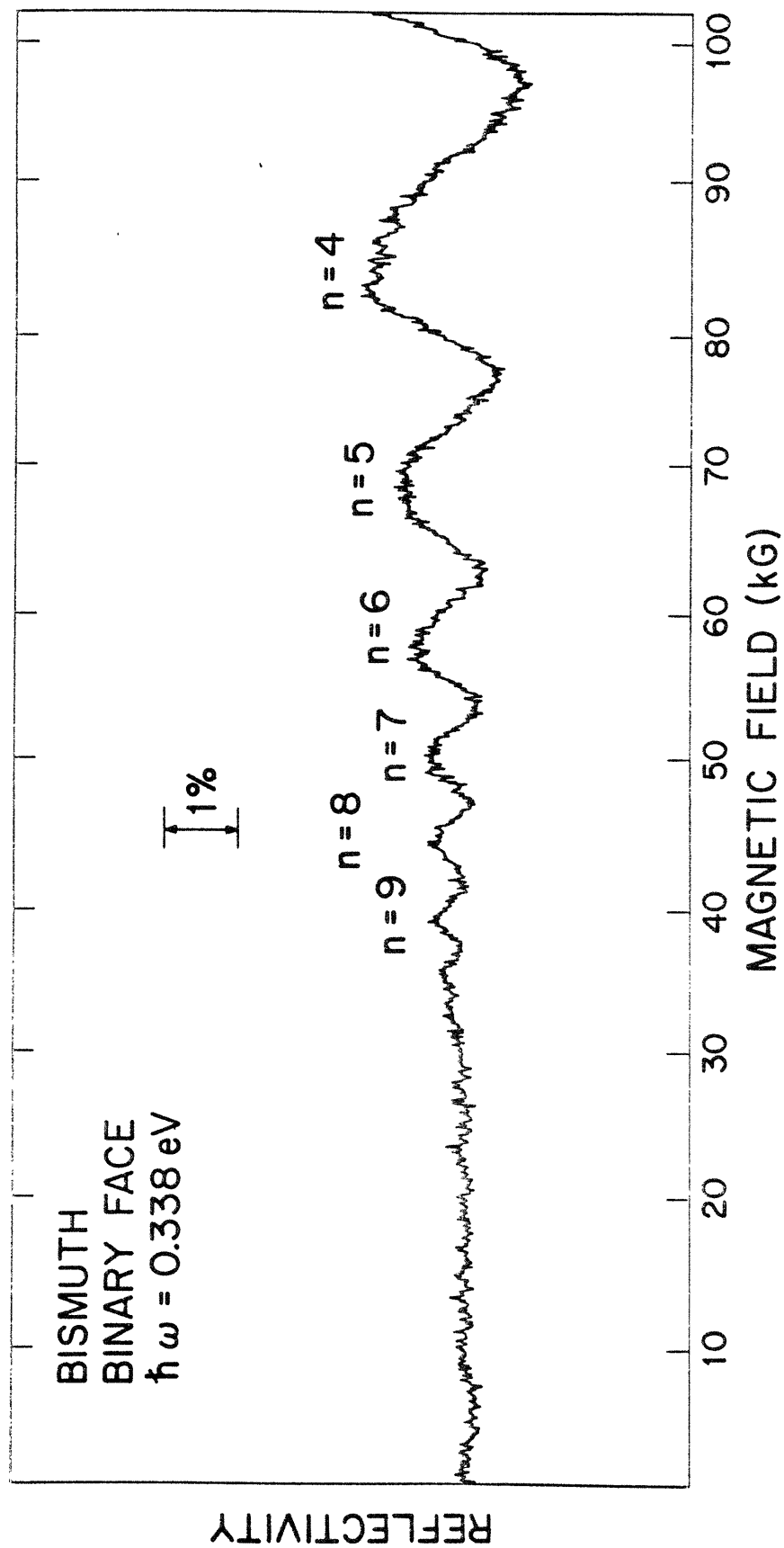
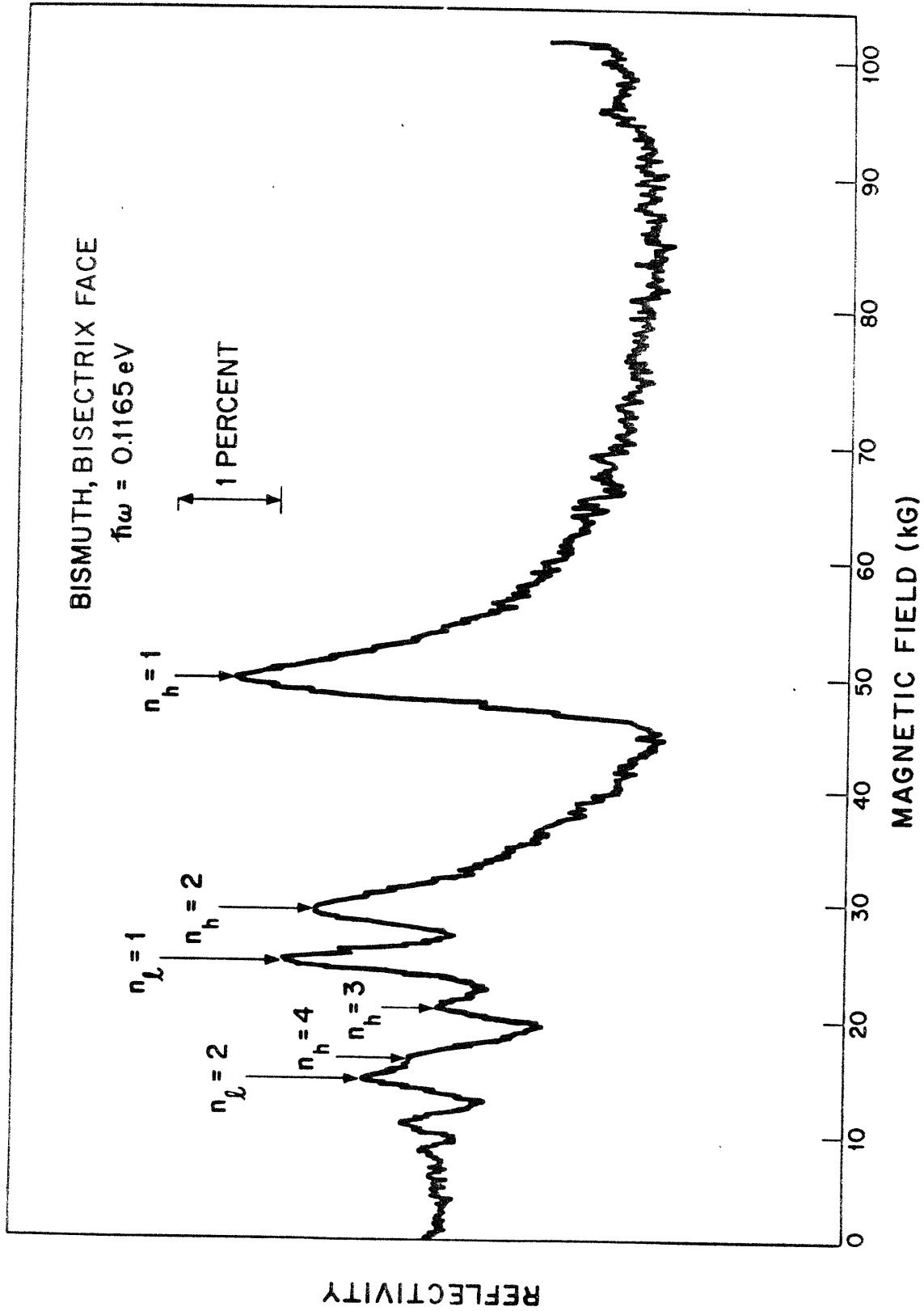


FIGURE 7



OUTPUT, ENHANCETRON COMPUTER USING 4 FULL TRACES

FIGURE 8a

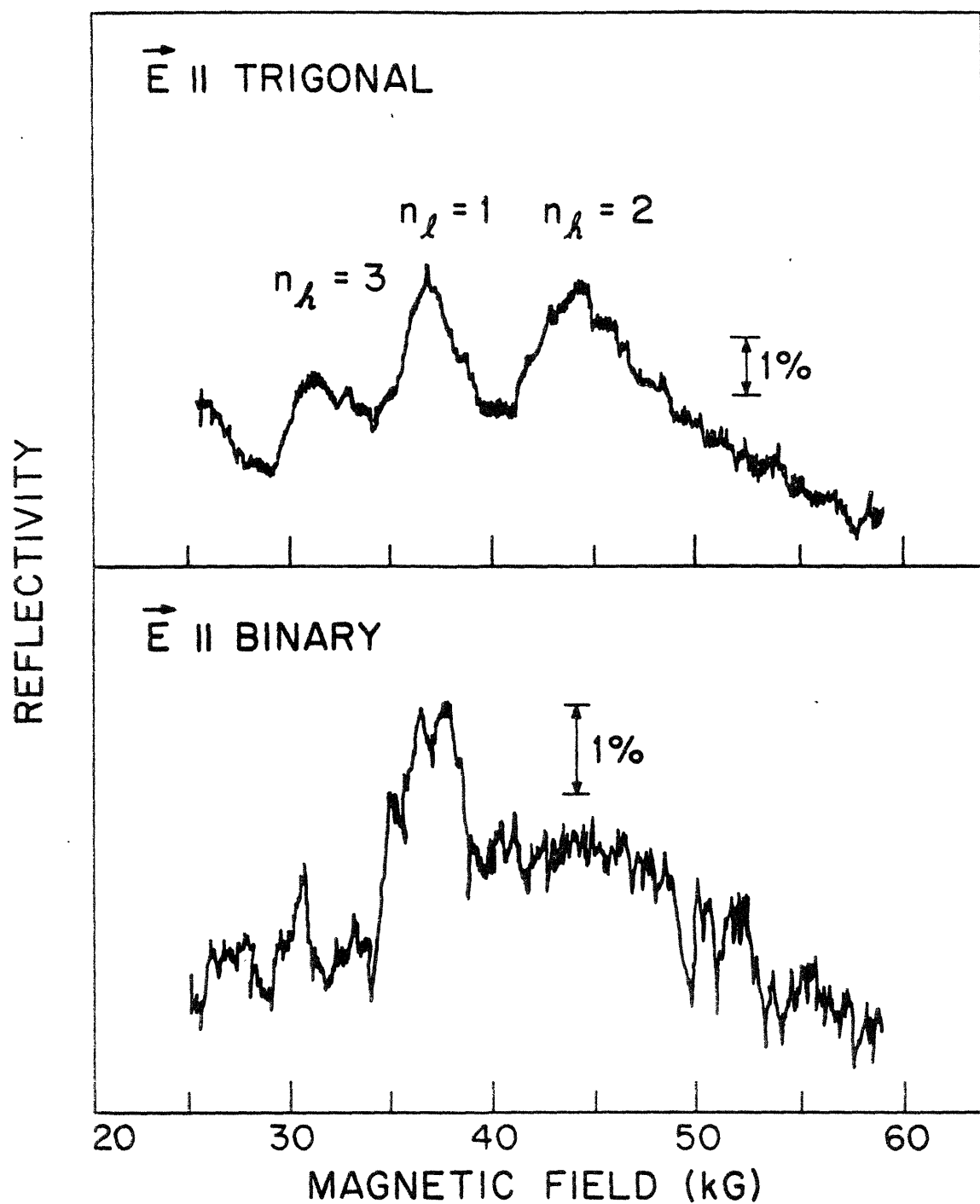
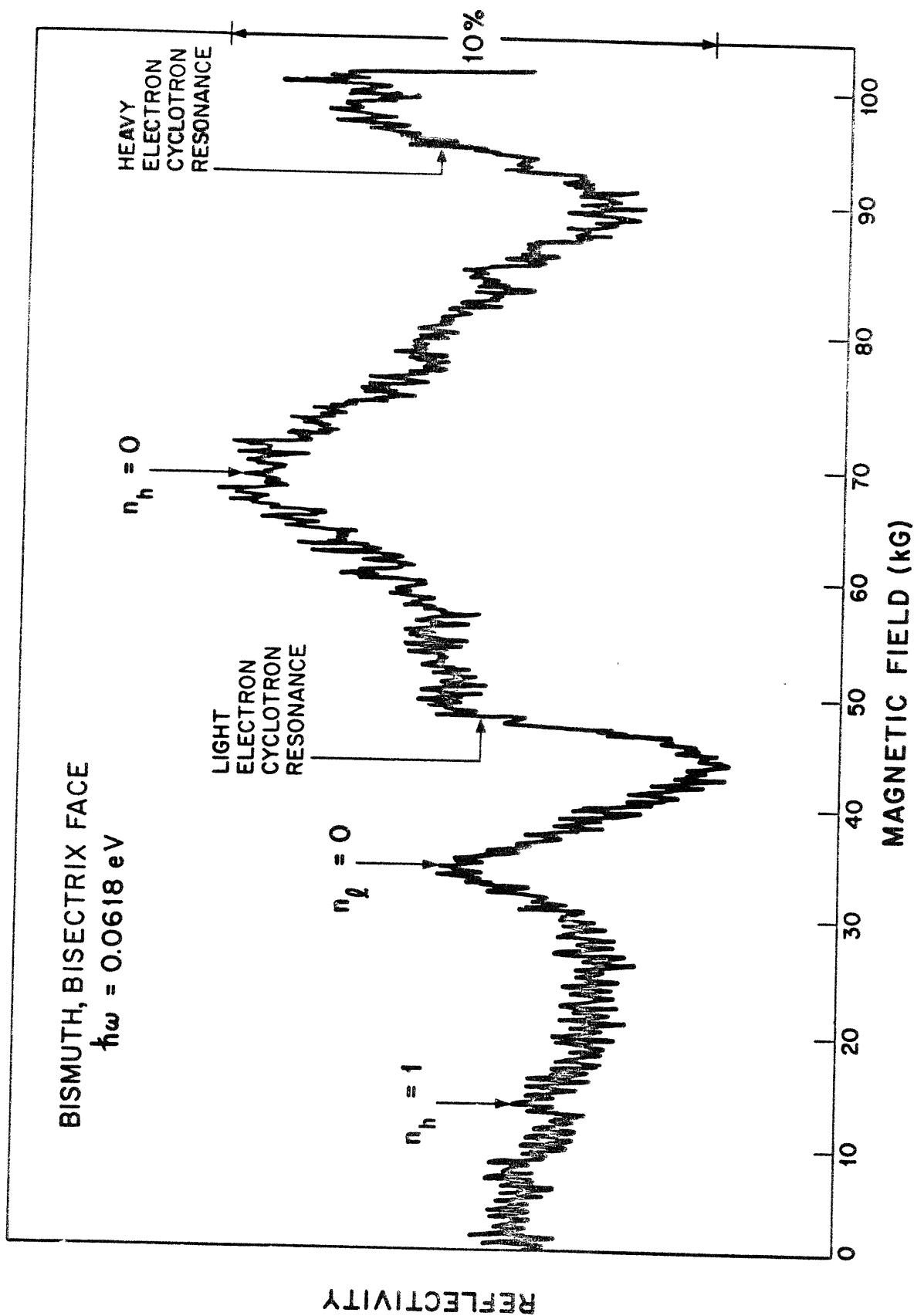


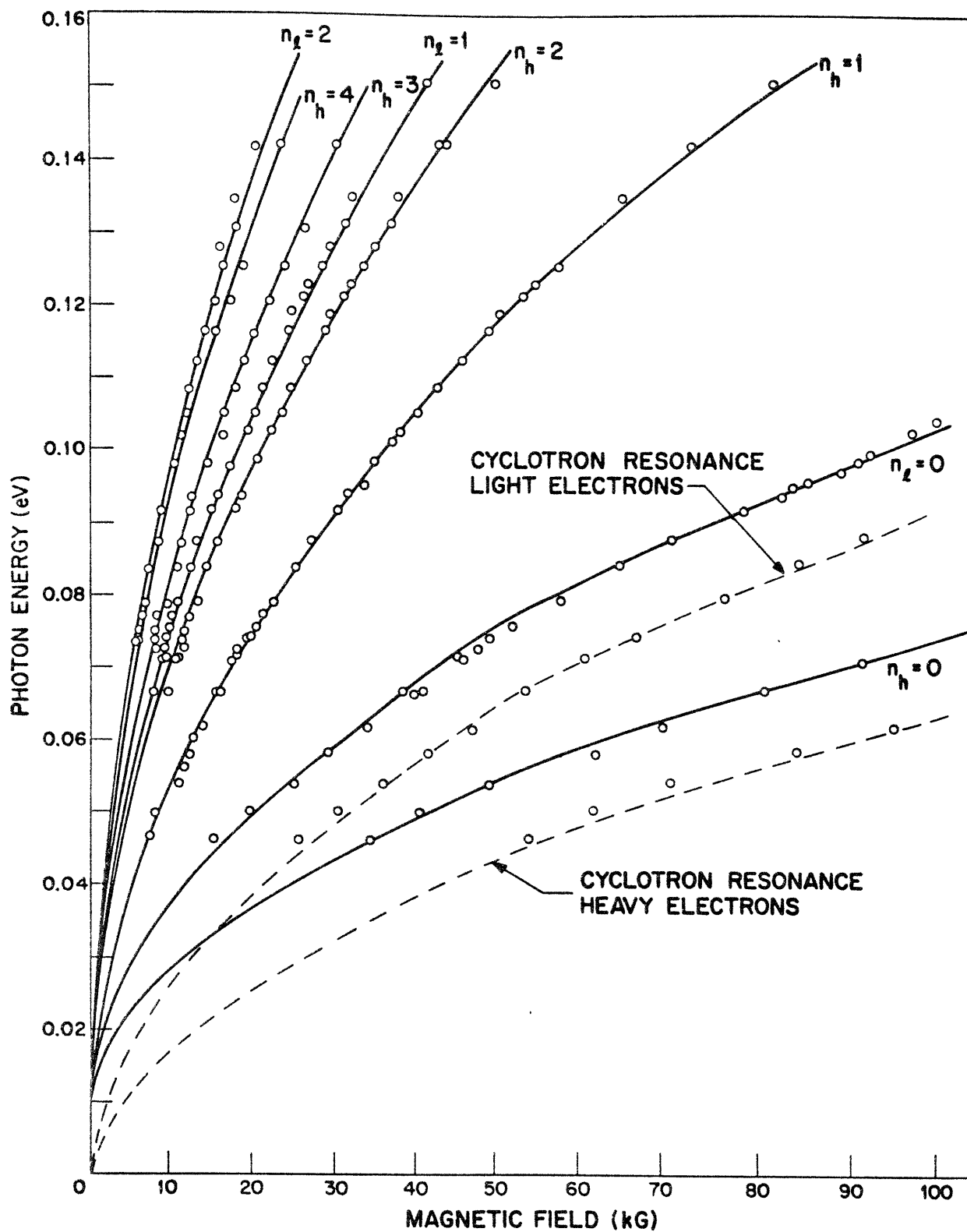
FIGURE 8b

BISMUTH, BISECTRIX FACE
 ($\hbar \omega = 0.1425 \text{ eV}$)



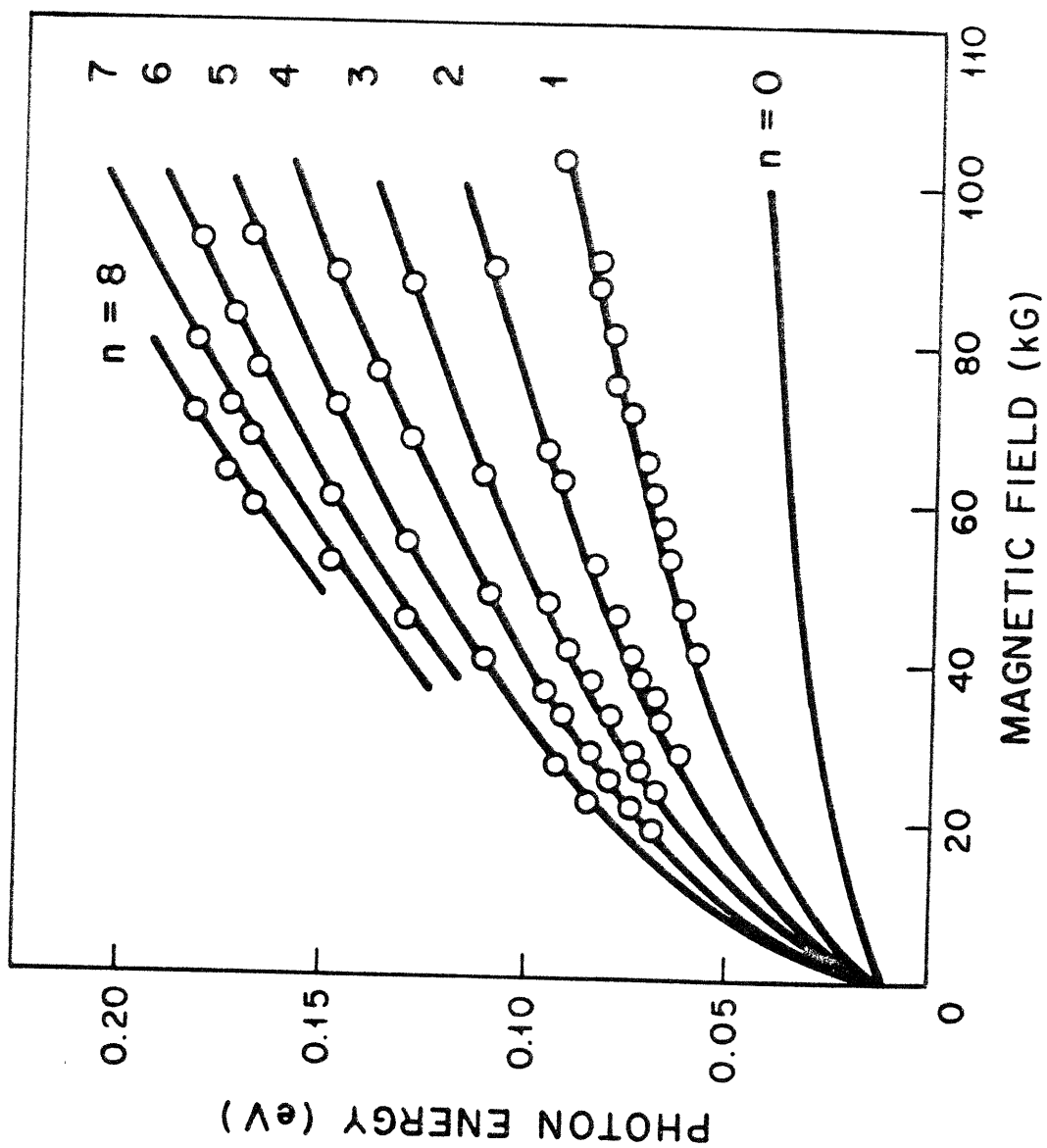
ENHANCETRON COMPUTER OUTPUT USING 2 FULL TRACES

FIGURE 9



EXPERIMENTAL AND THEORETICAL RESONANCES
BISMUTH BISECTRIX FACE

FIGURE 10



BISMUTH TRIGONAL FACE
REFLECTIVITY PEAKS

FIGURE 11

BARAFF MODEL

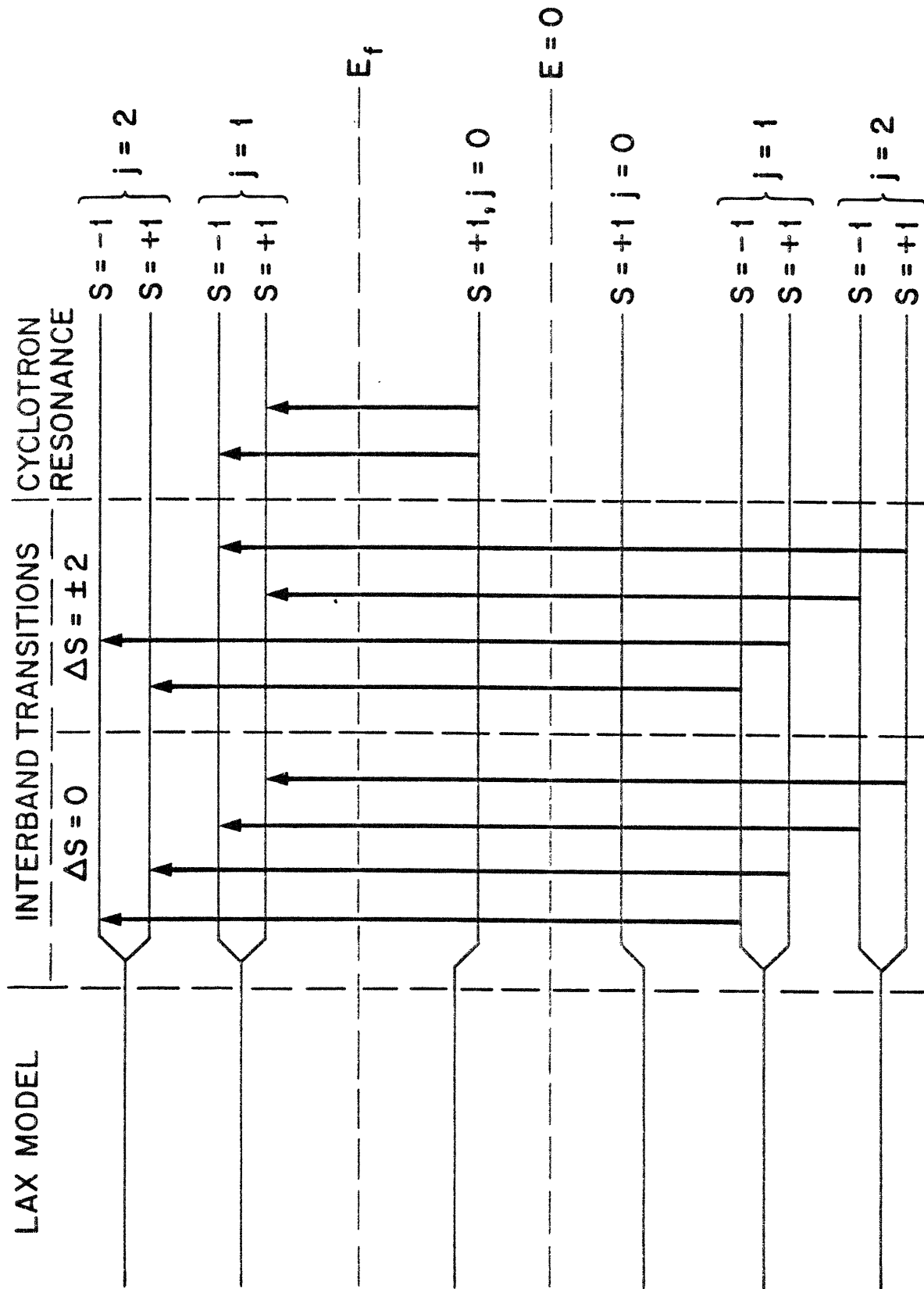


FIGURE 12

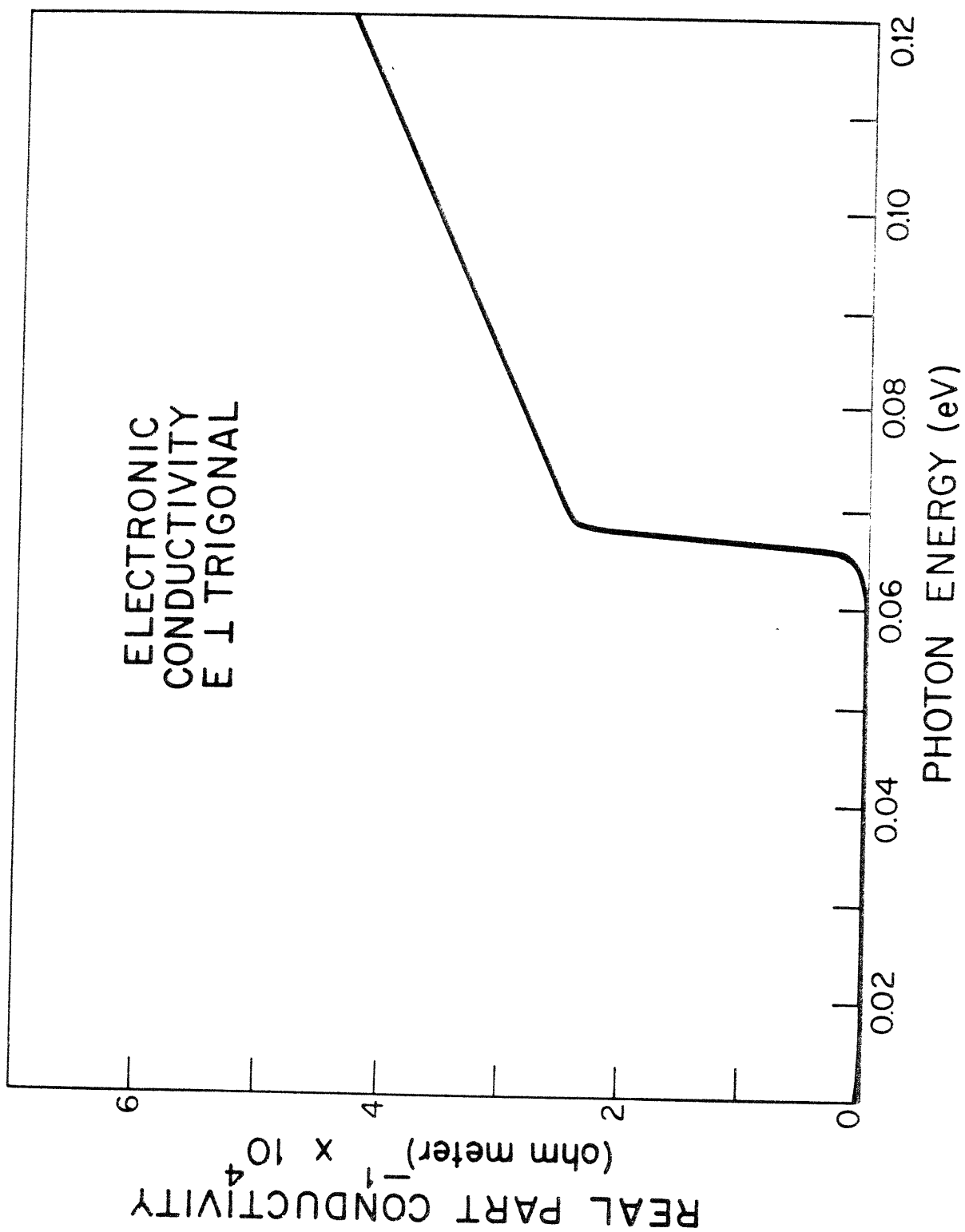


FIGURE 13a

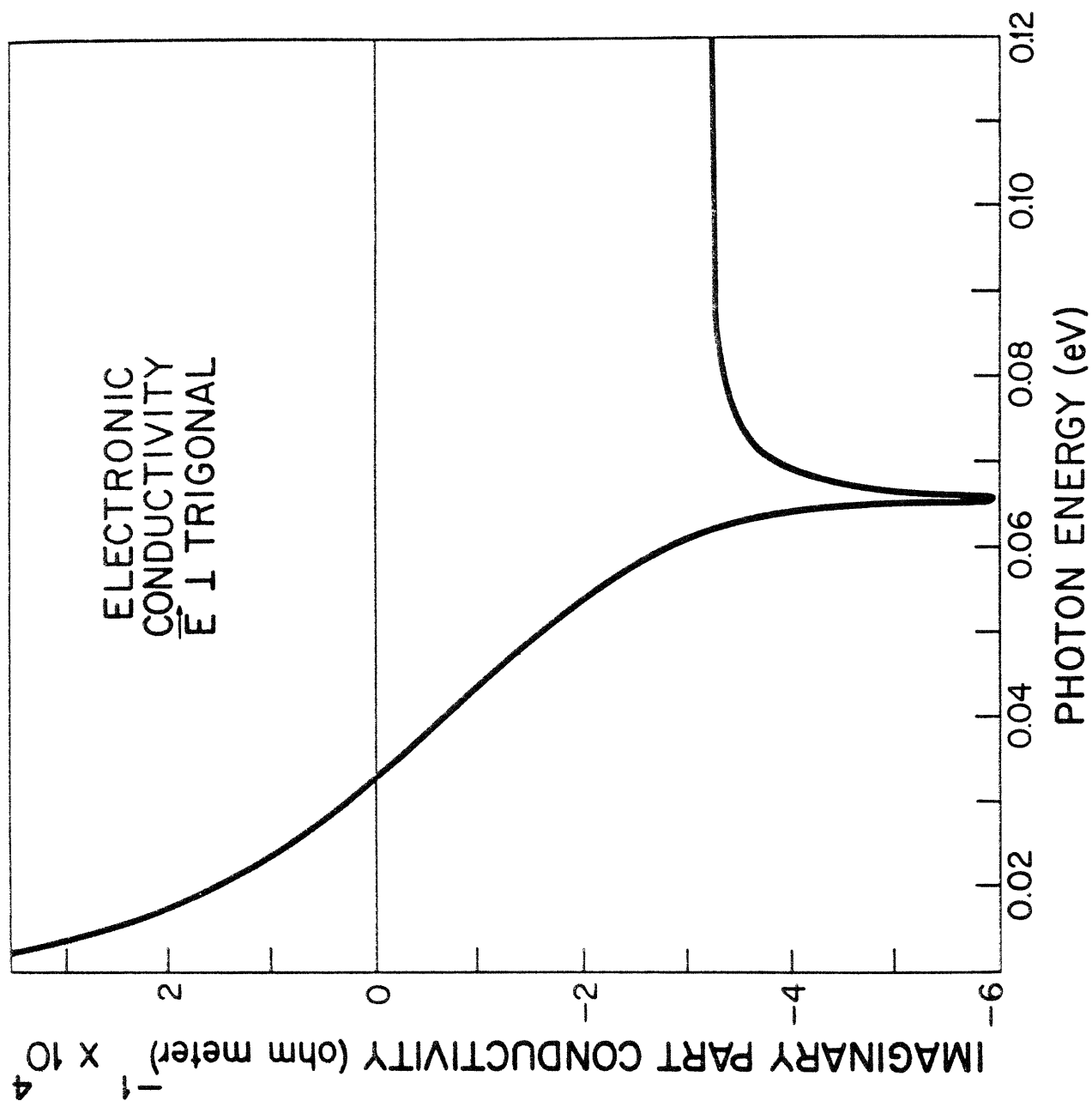


FIGURE 13b

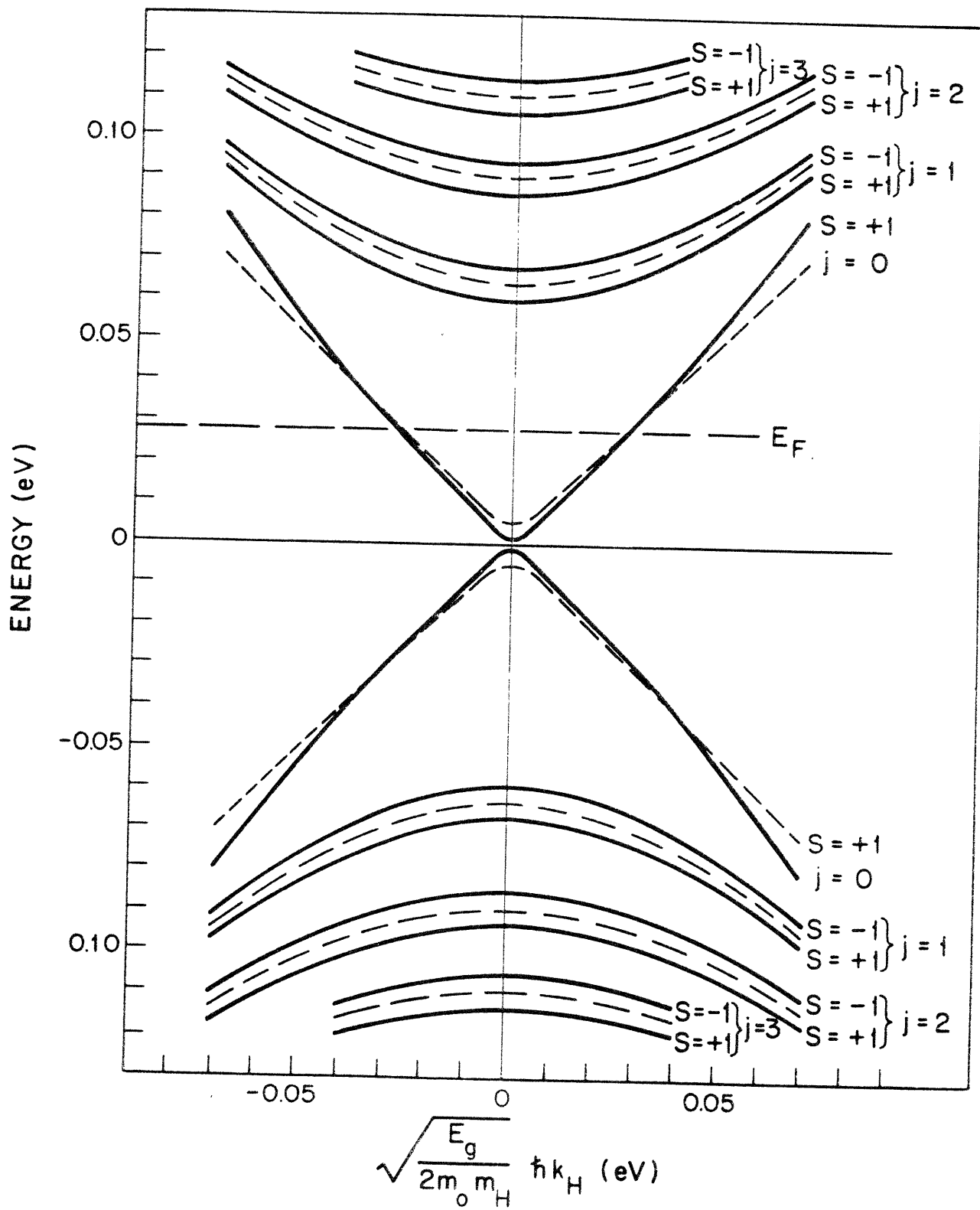


FIGURE 14

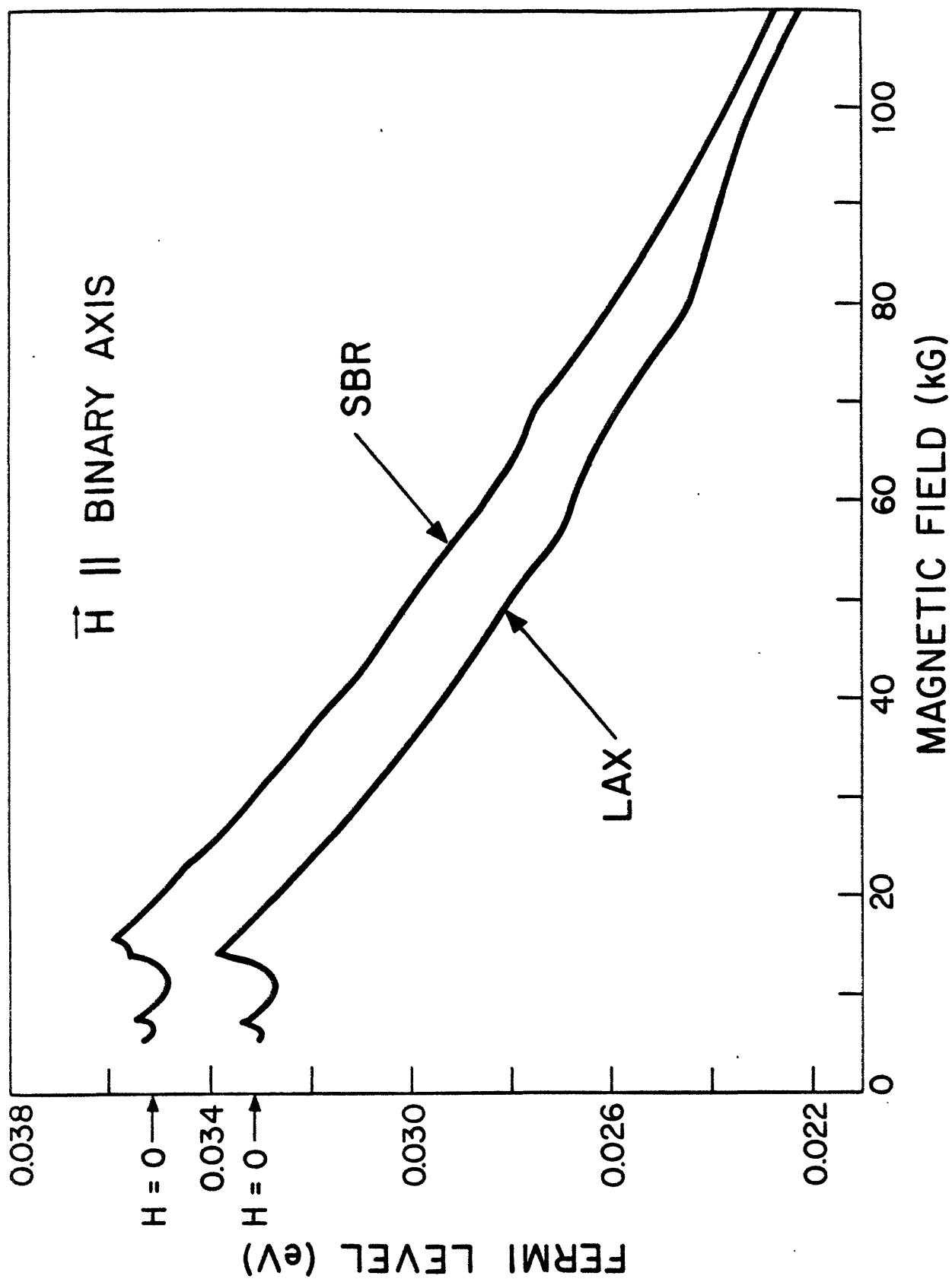


FIGURE 15

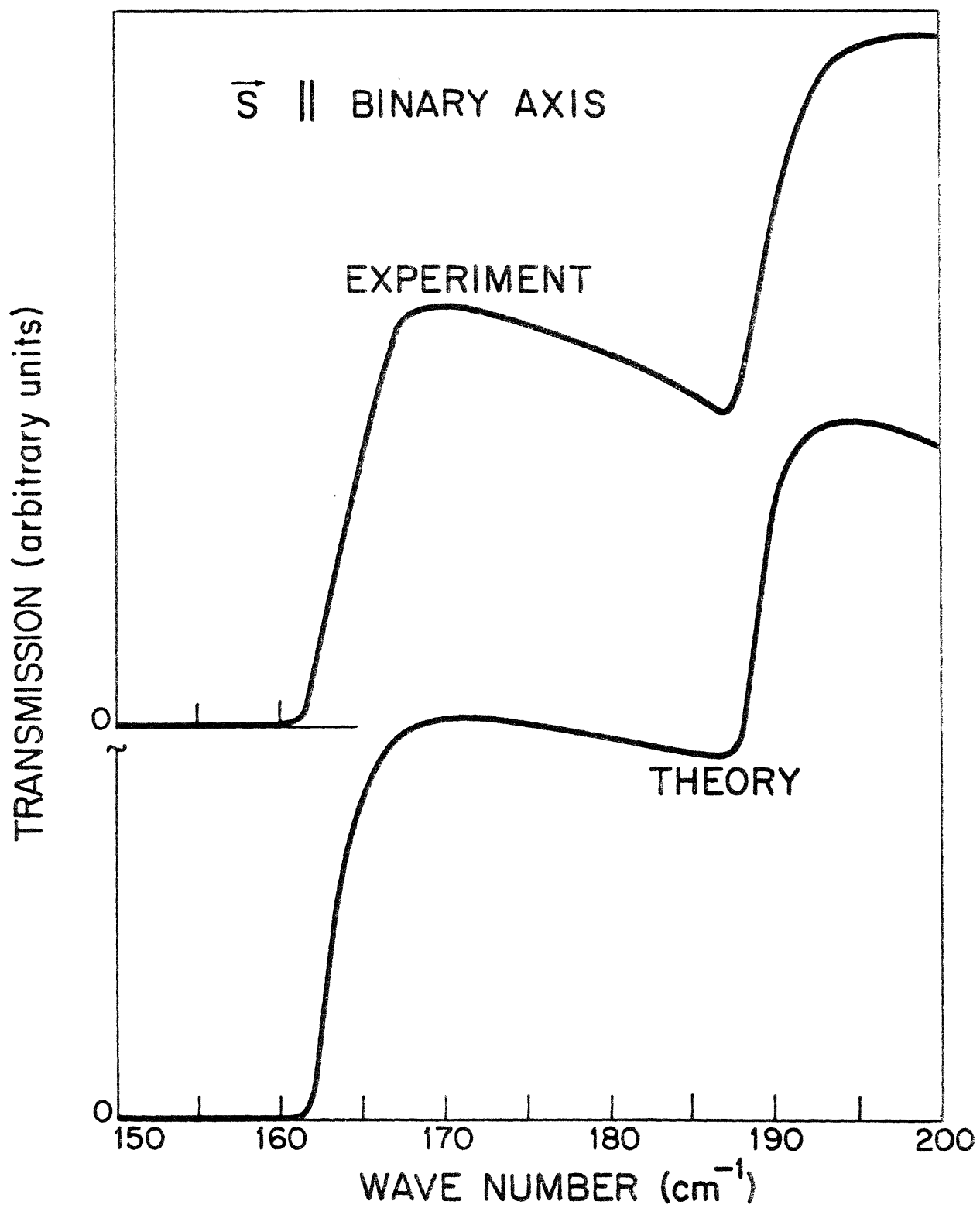


FIGURE 16

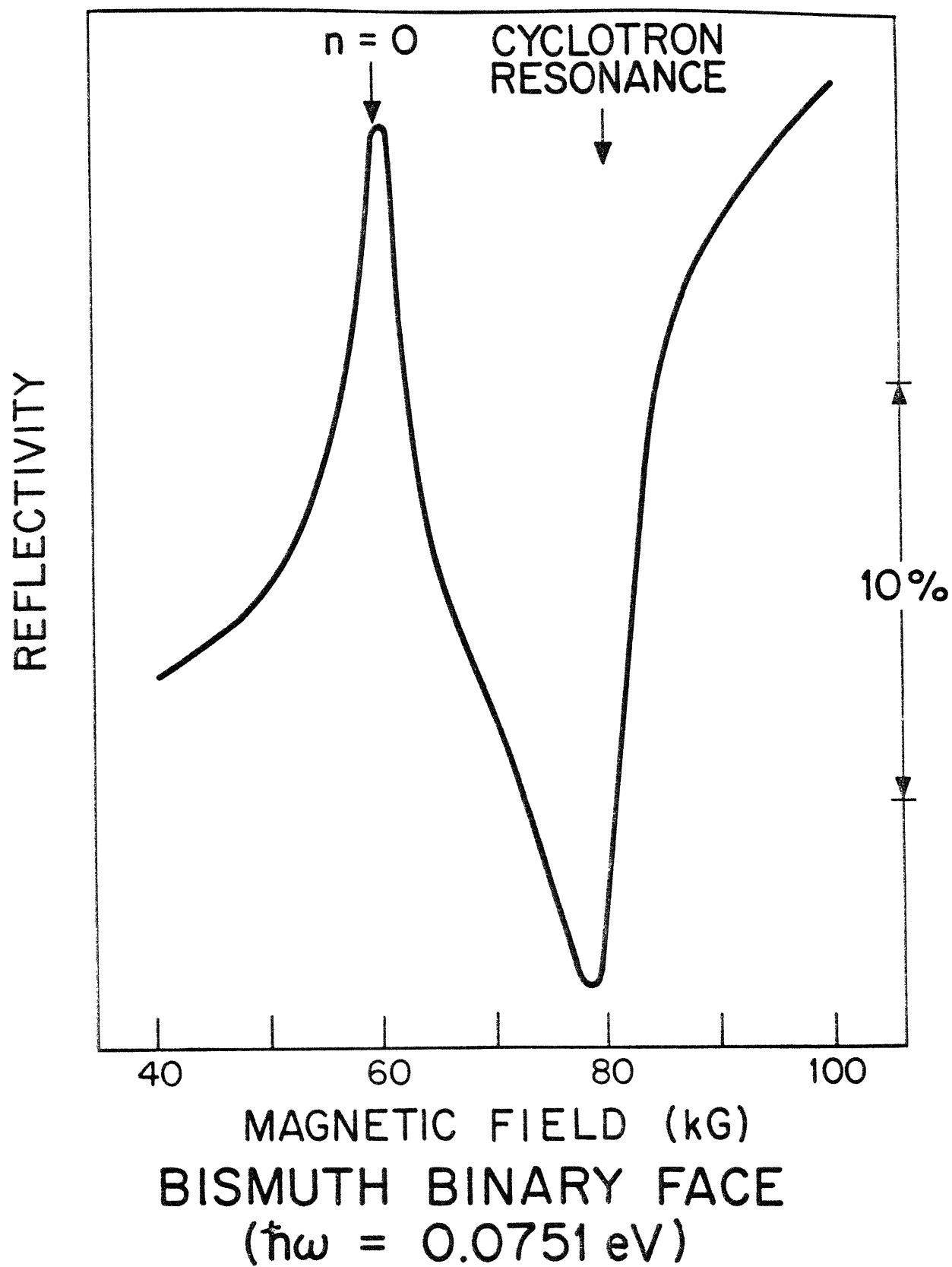


FIGURE 17

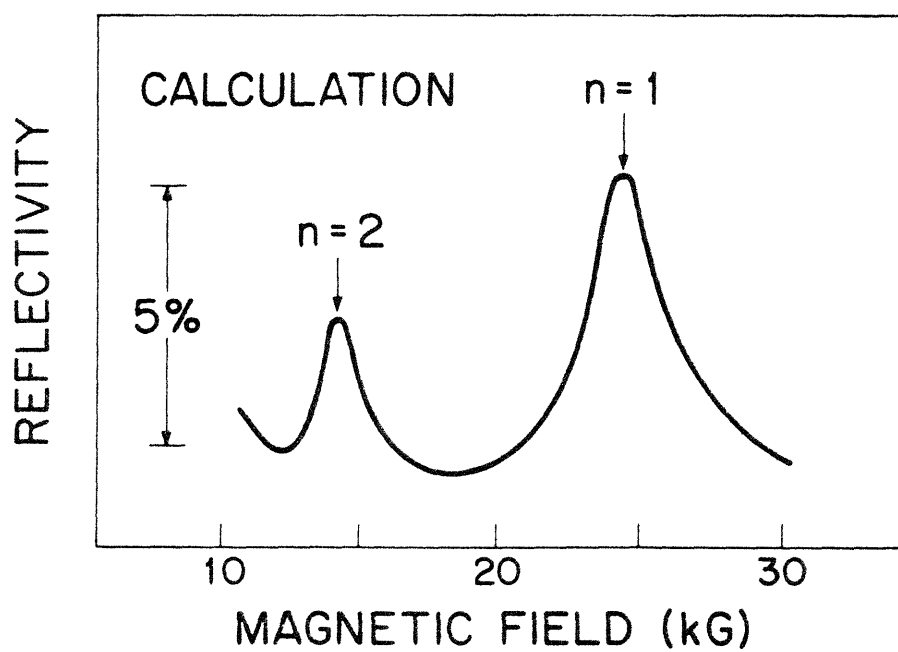
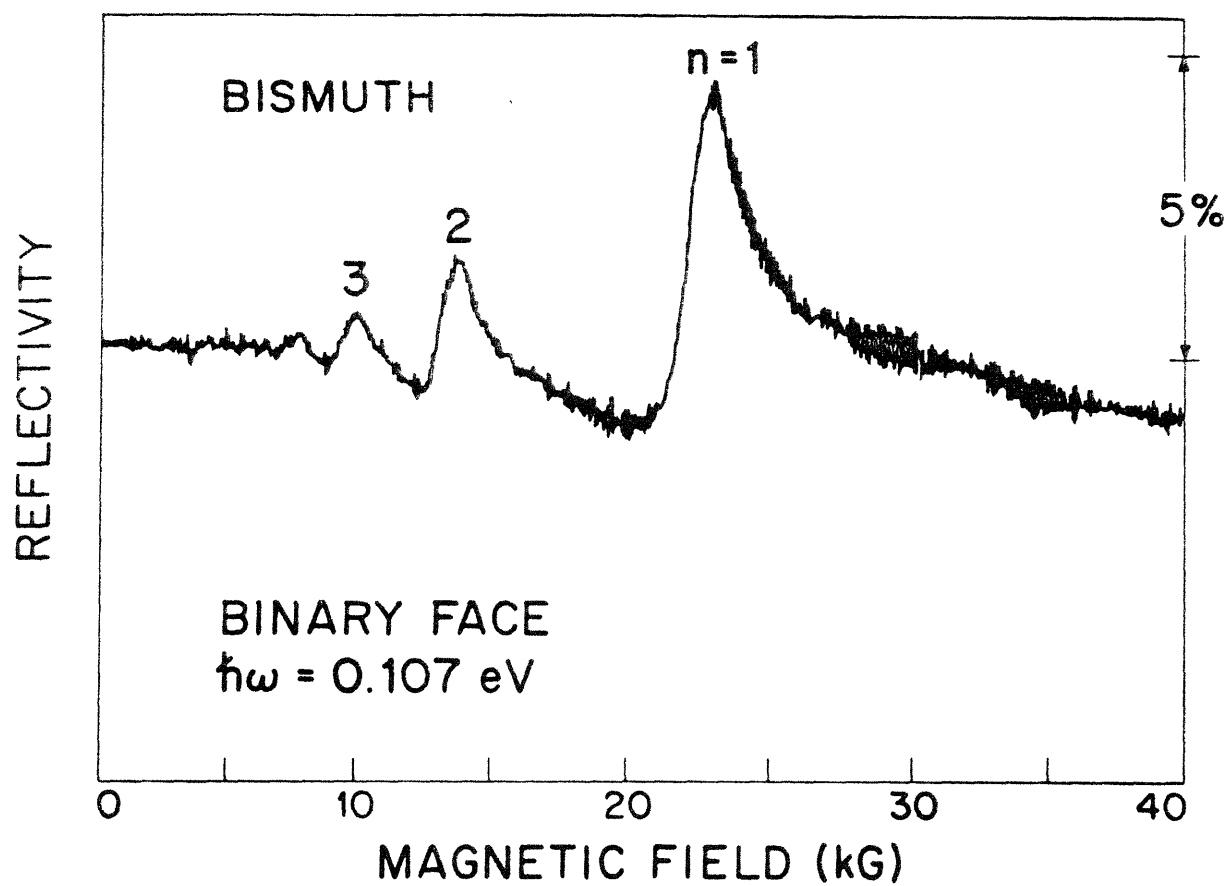


FIGURE 18

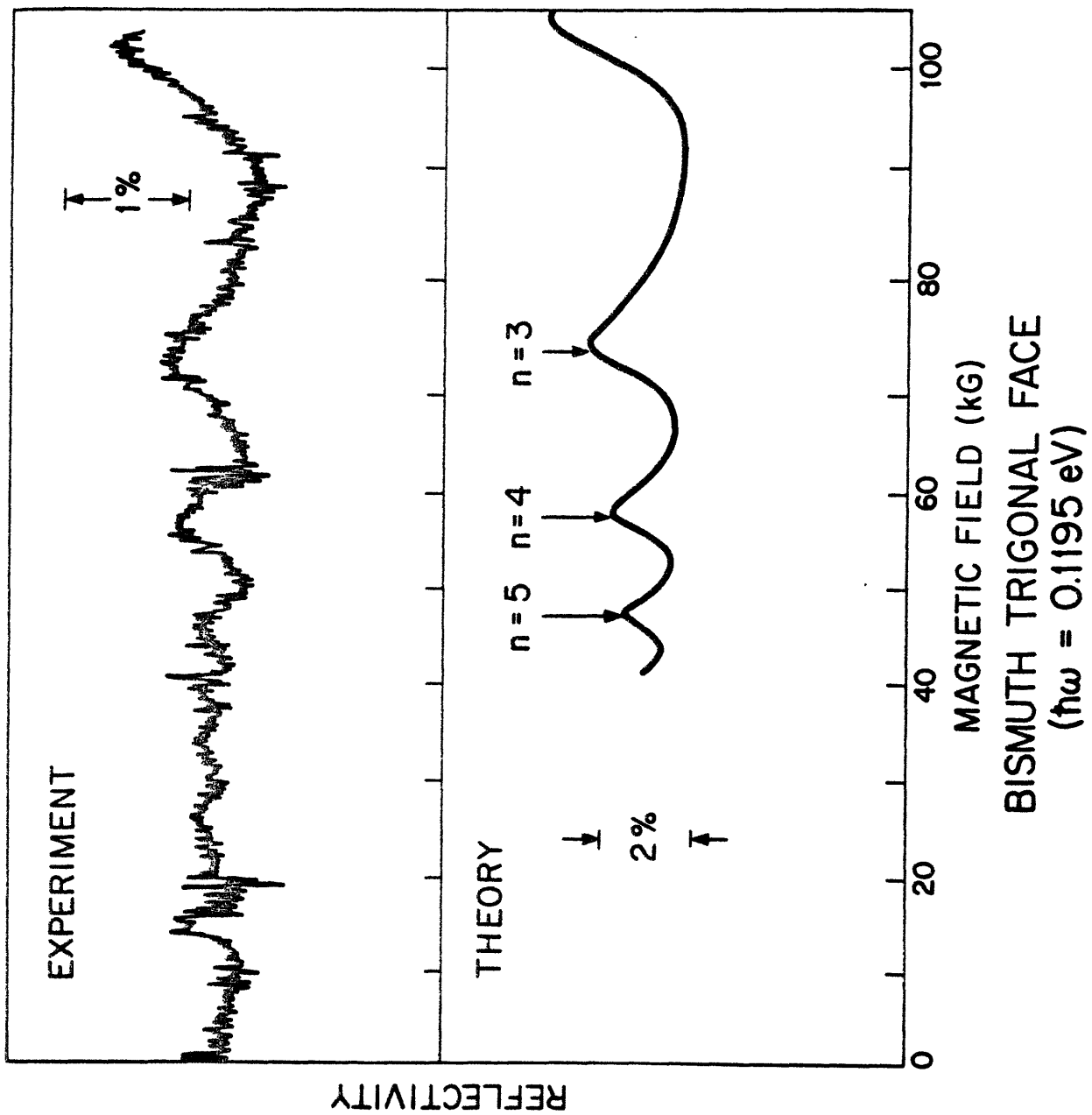
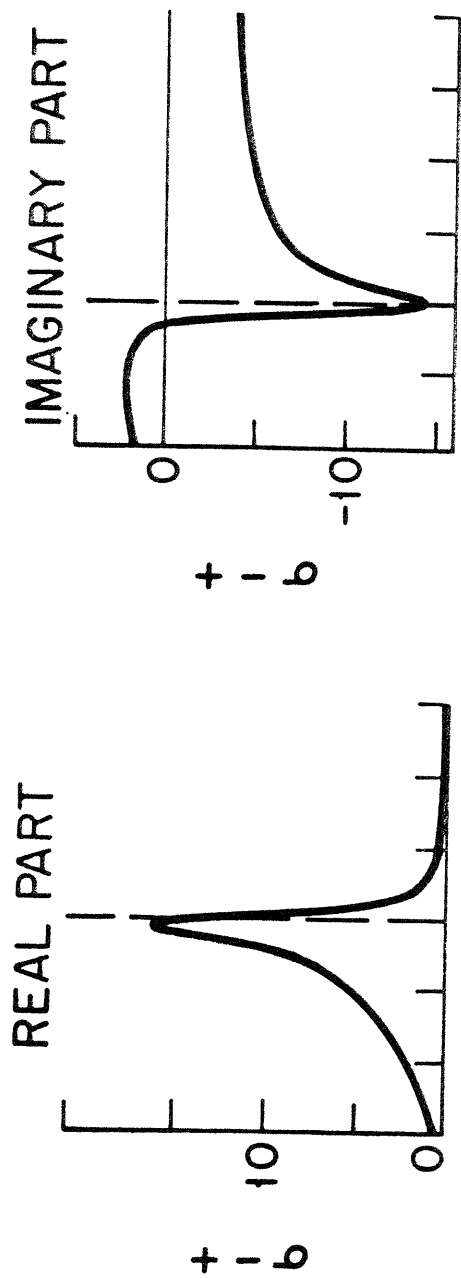
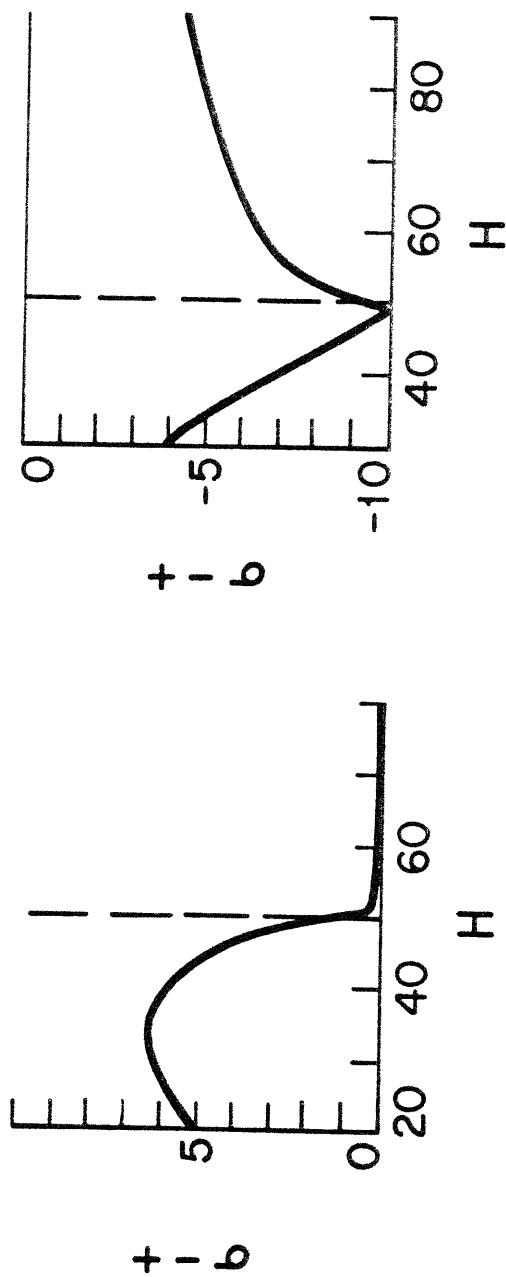


FIGURE 19

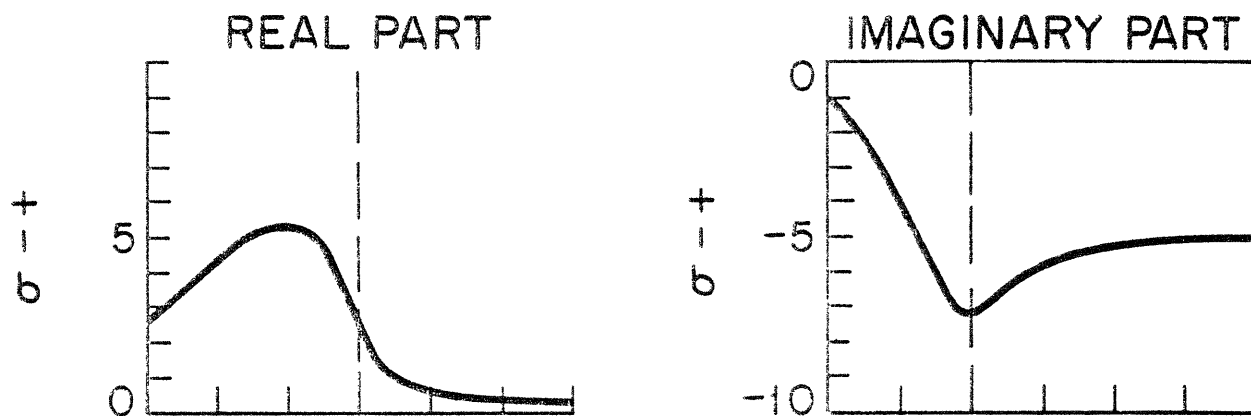


(a) NORMAL SPIN CONSERVING

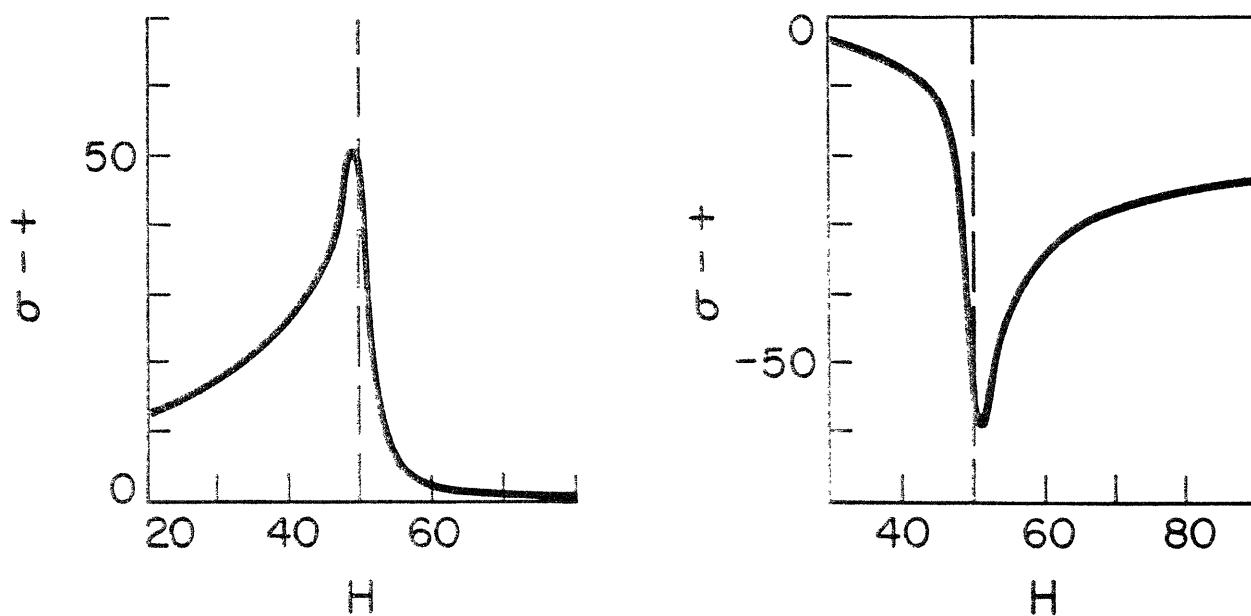


(b) NORMAL SPIN FLIPPING

FIGURE 20a&b

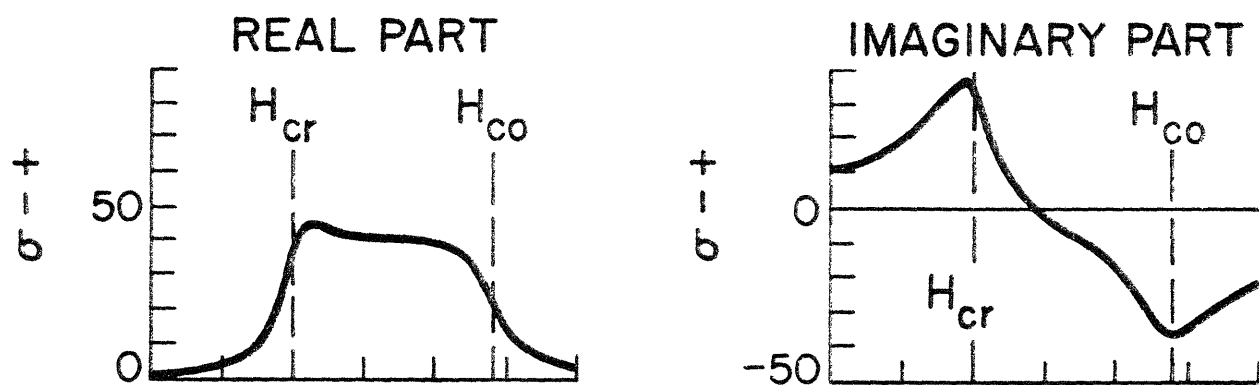


(c) ANOMALOUS SPIN CONSERVING

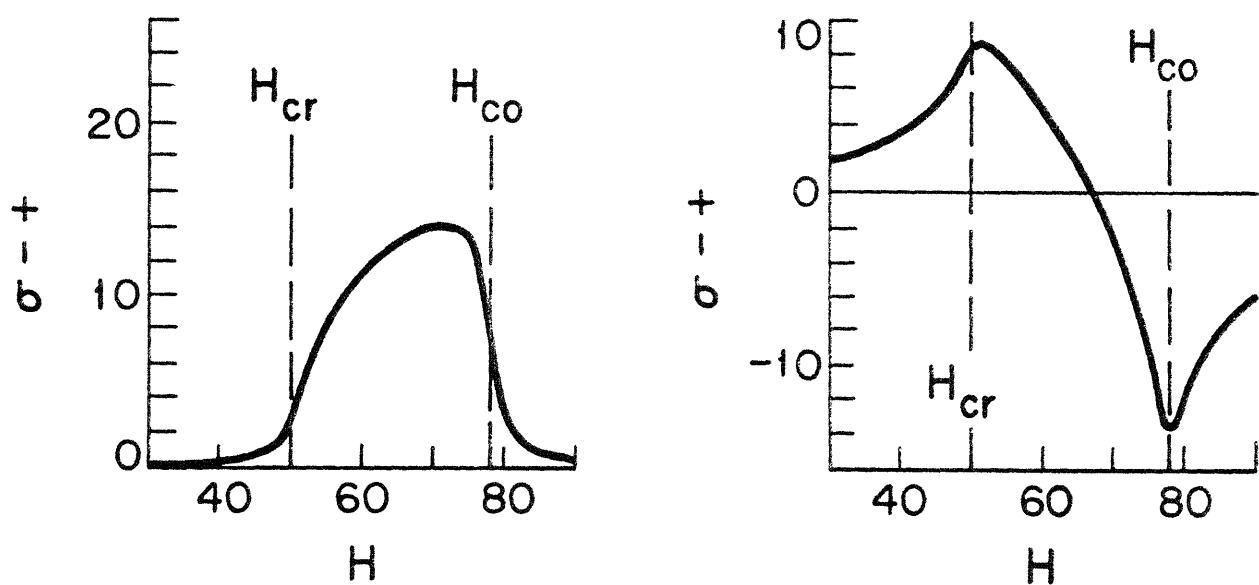


(d) ANOMALOUS SPIN FLIPPING

FIGURE 20c&d



(e) SPIN-CONSERVING INTRABAND



(f) SPIN-FLIPPING INTRABAND

FIGURE 20e&f

NORMALIZED VELOCITY MATRIX ELEMENT SQUARED

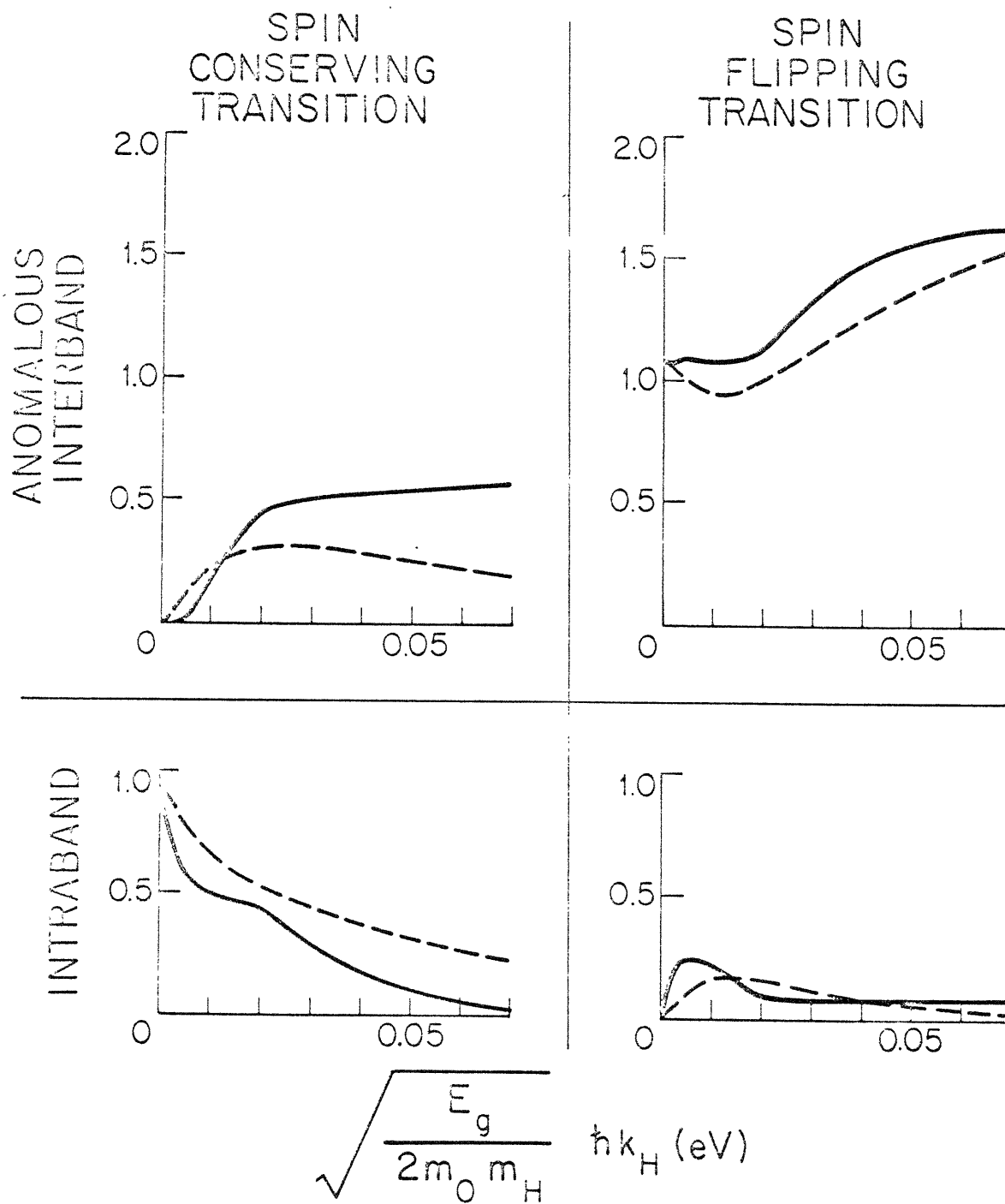
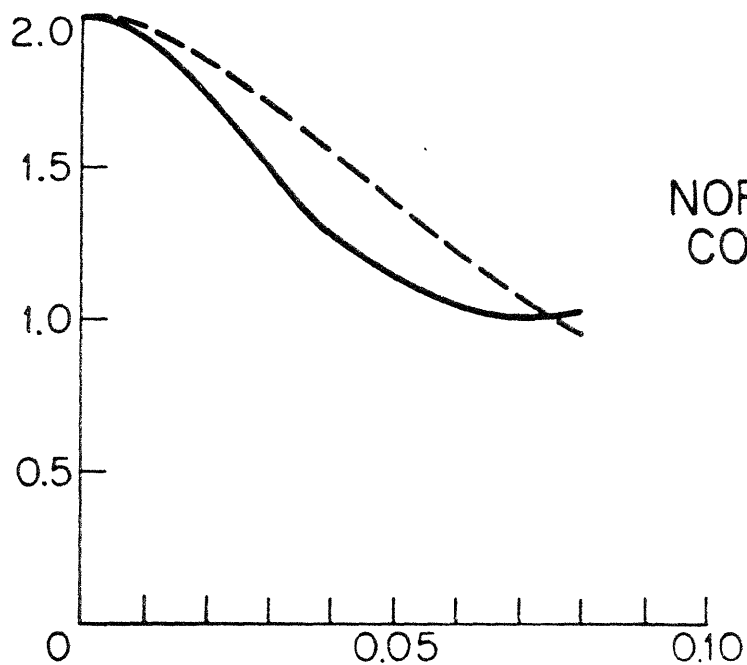


FIGURE 21a

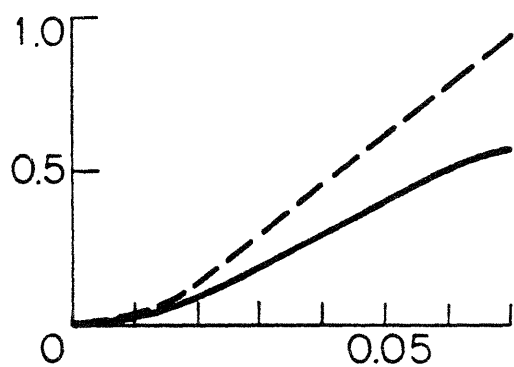
NORMALIZED VELOCITY MATRIX ELEMENT SQUARED



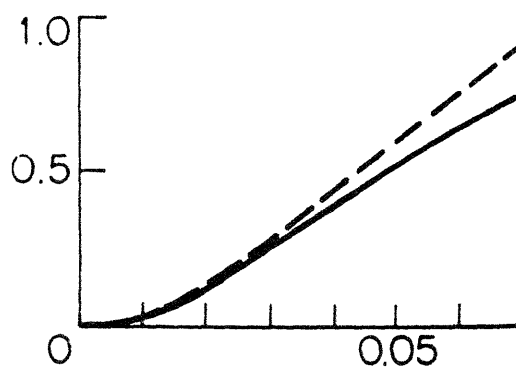
NORMAL SPIN
CONSERVING

NORMAL SPIN
FLIPPING

SHIFTED
UP



SHIFTED
DOWN



$$\sqrt{\frac{E_g}{2m_0 m_H}} \hbar k_H \text{ (eV)}$$

FIGURE 21b

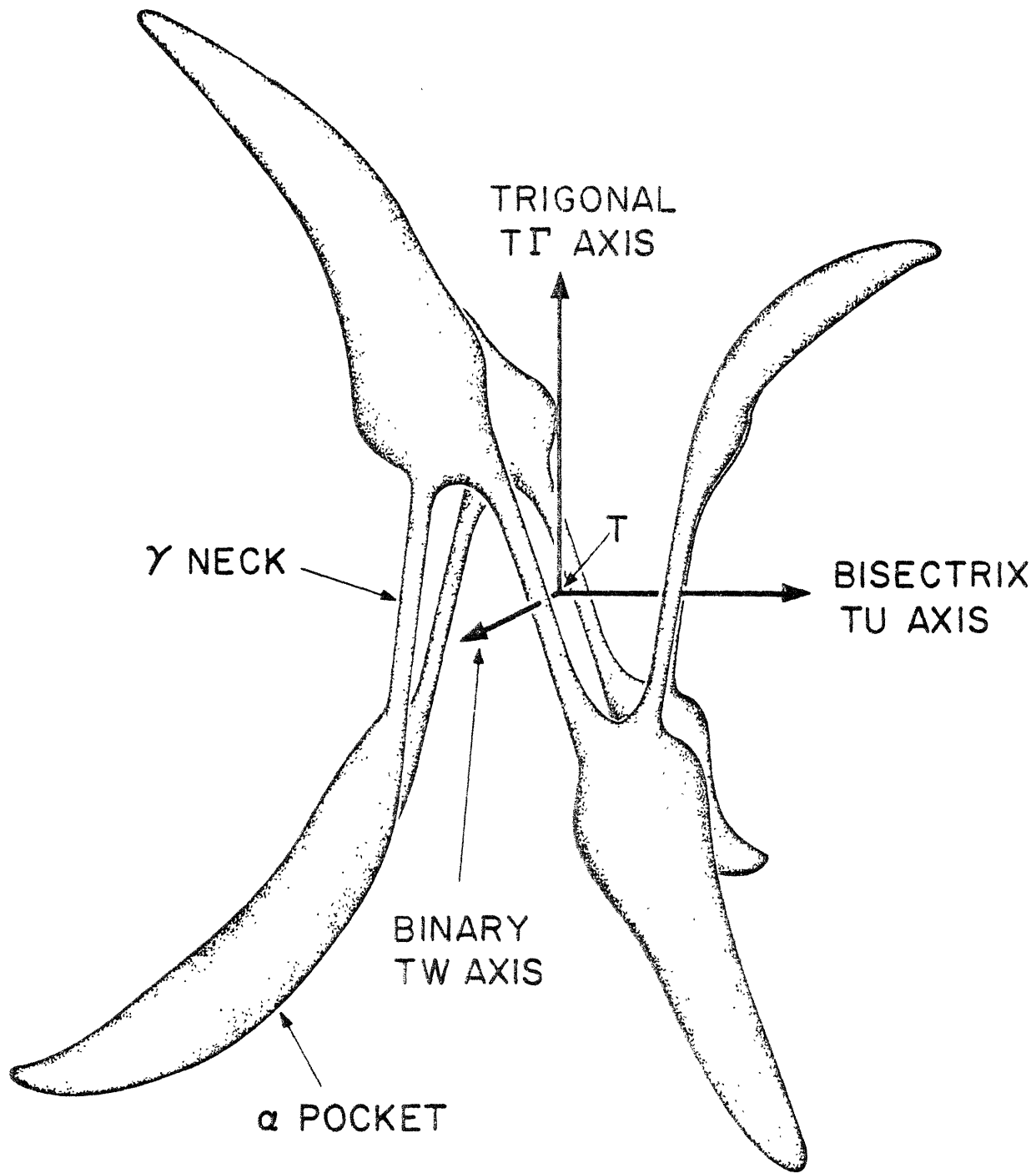
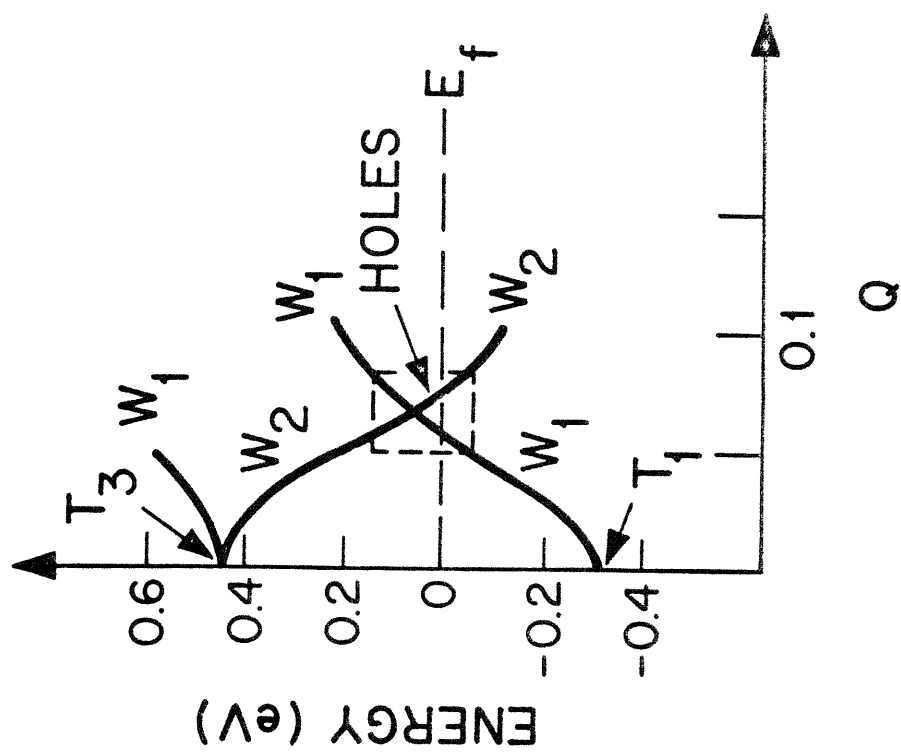


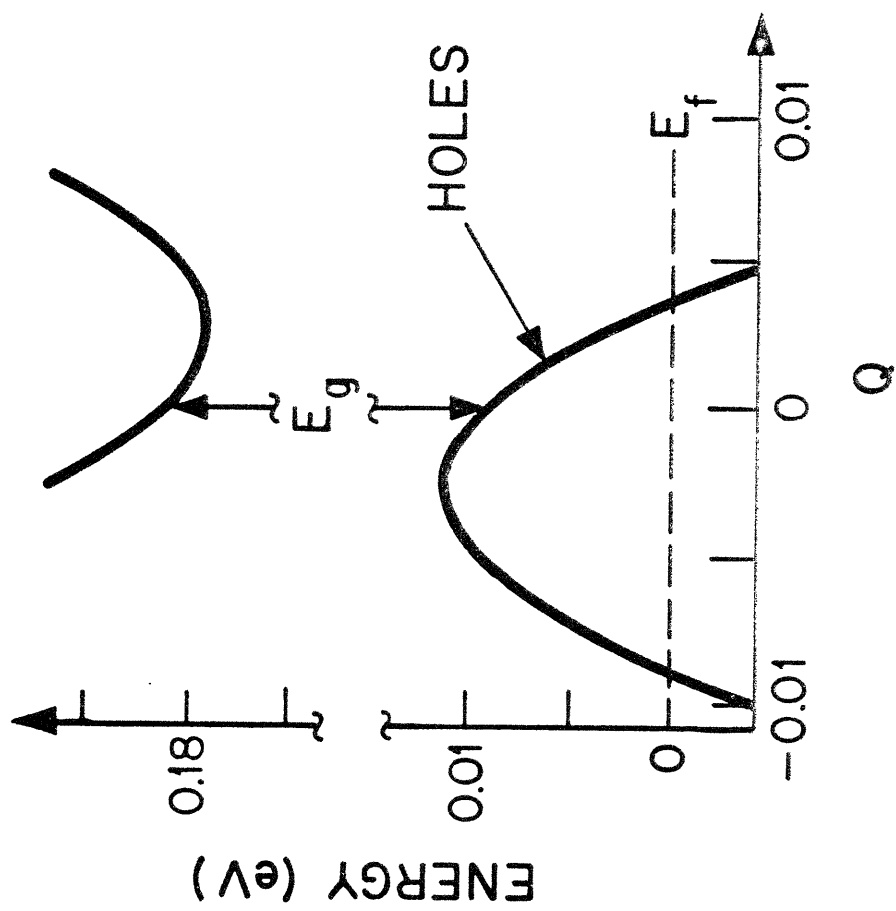
FIGURE 22

ARSENIC HOLE FERMI SURFACE

NO SPIN SPLITTING



SPIN SPLITTING



ENERGY BANDS NEAR γ NECK

FIGURE 23

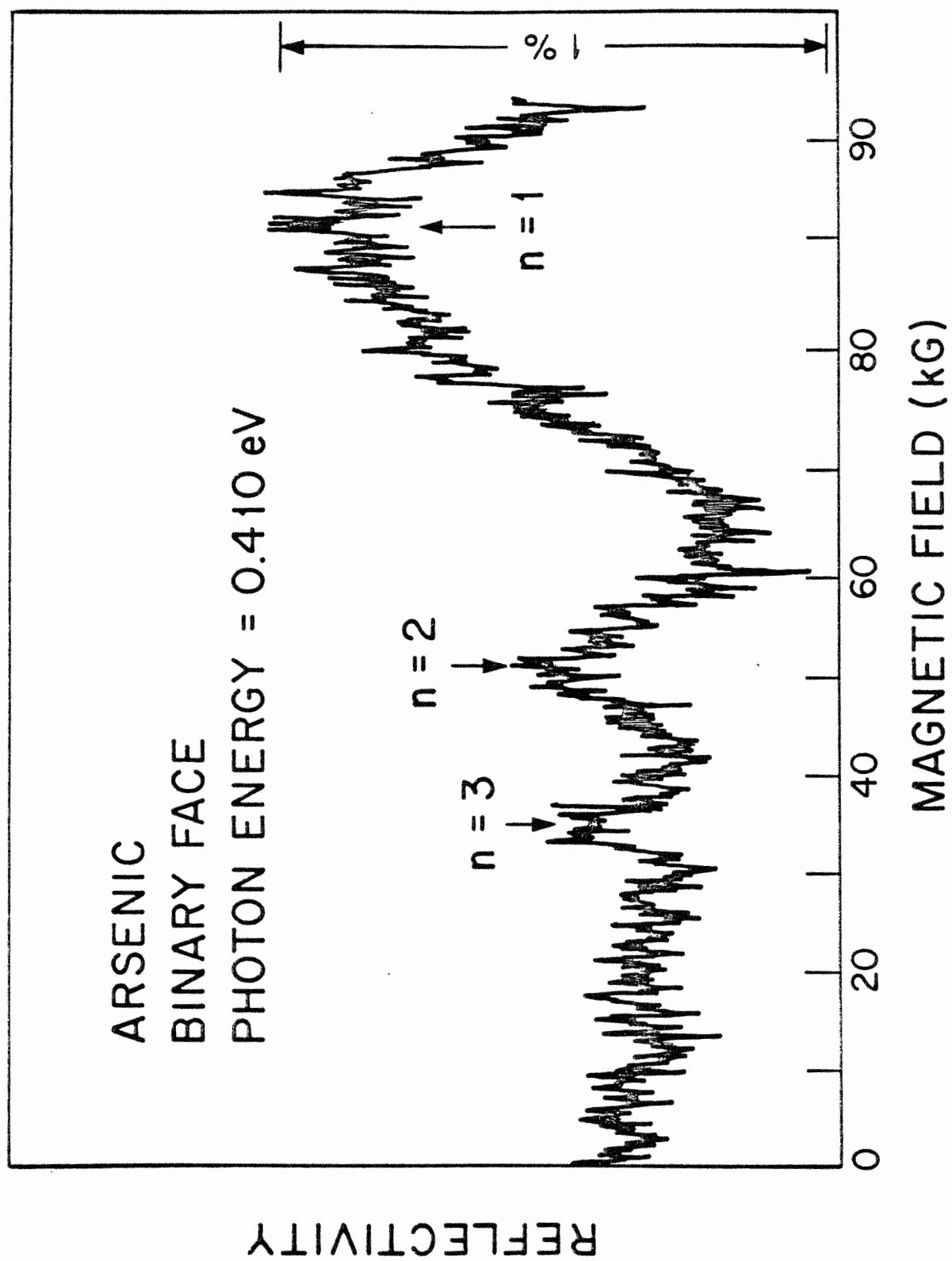


FIGURE 24

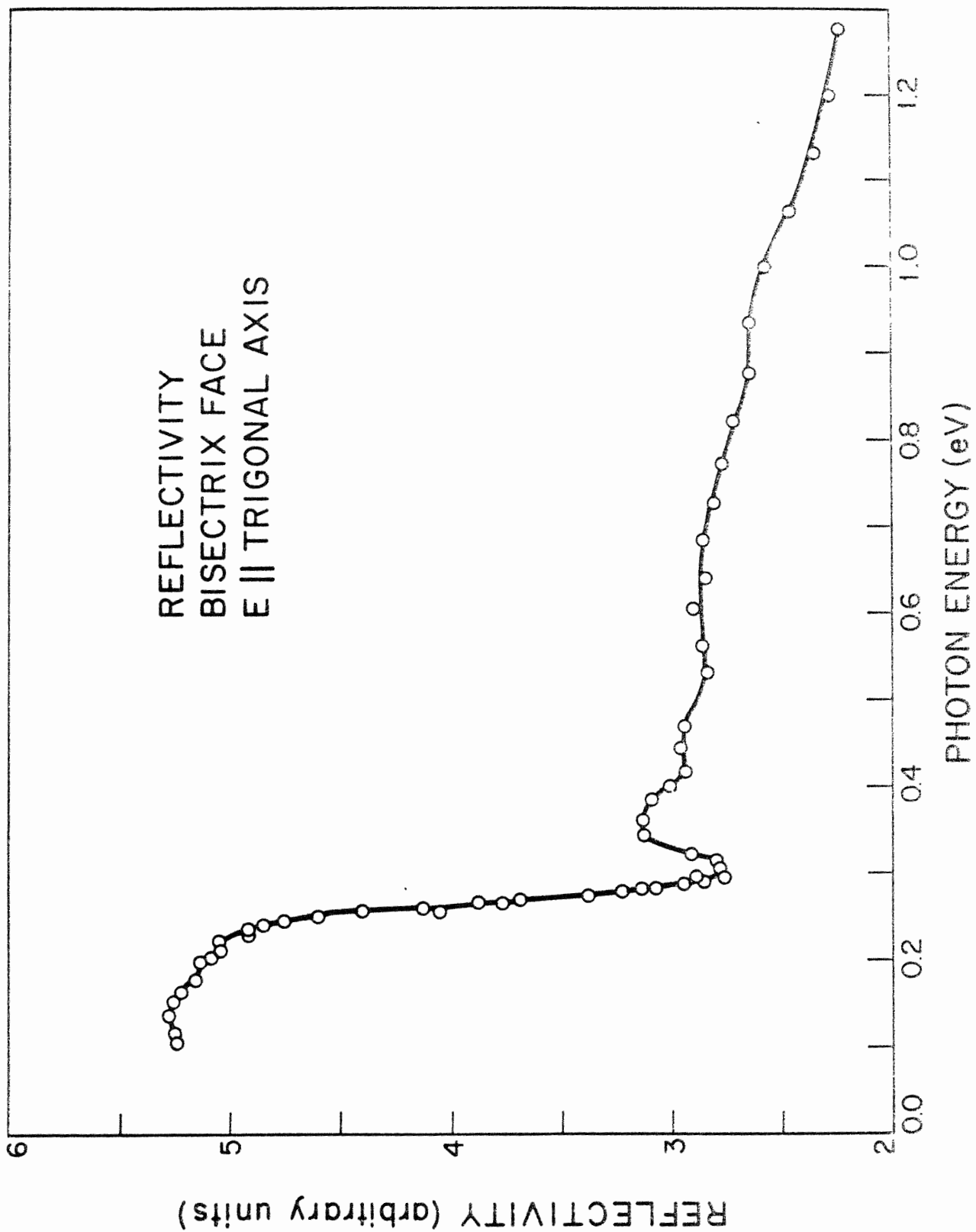


FIGURE 25

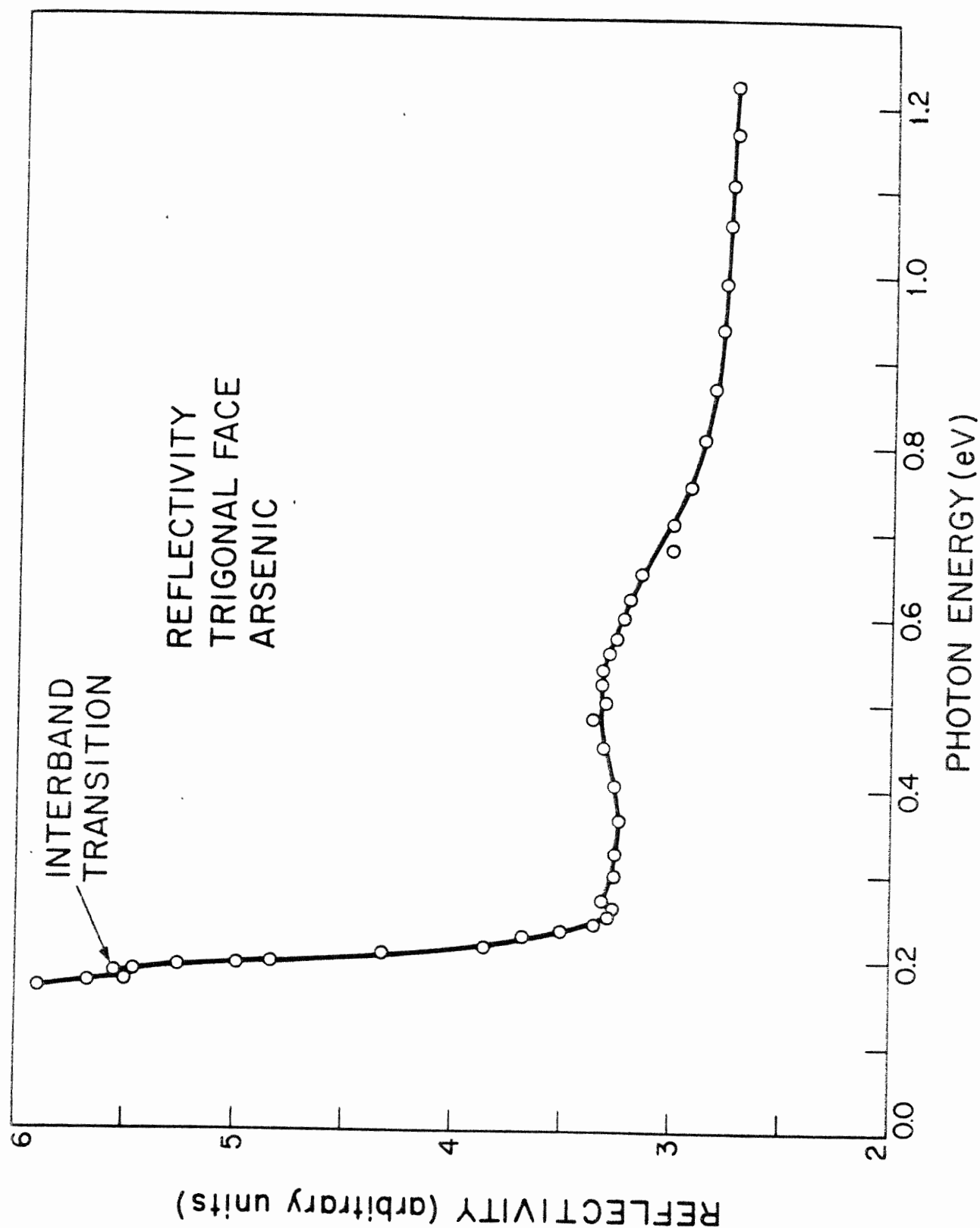


FIGURE 26

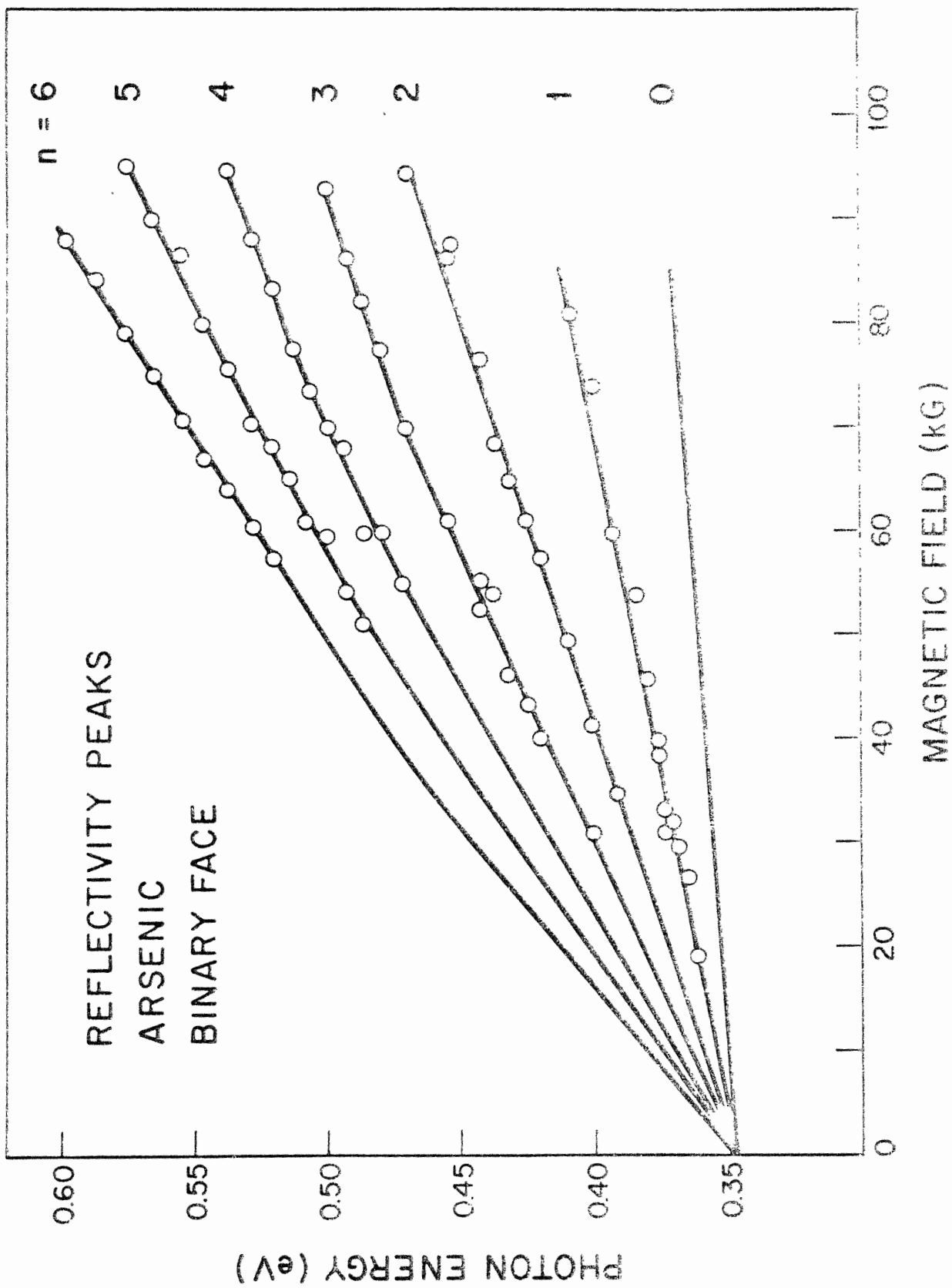


FIGURE 27

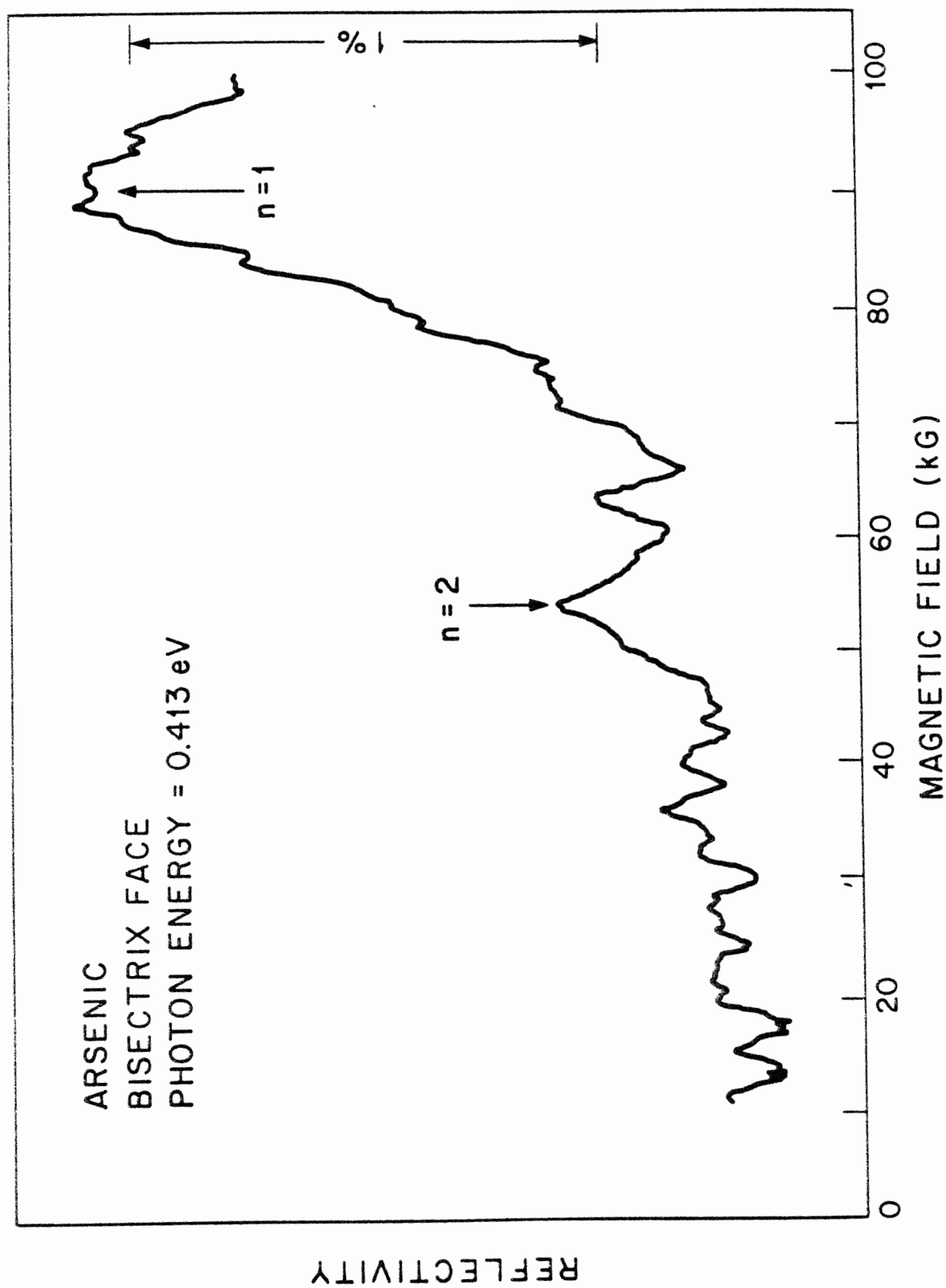


FIGURE 28

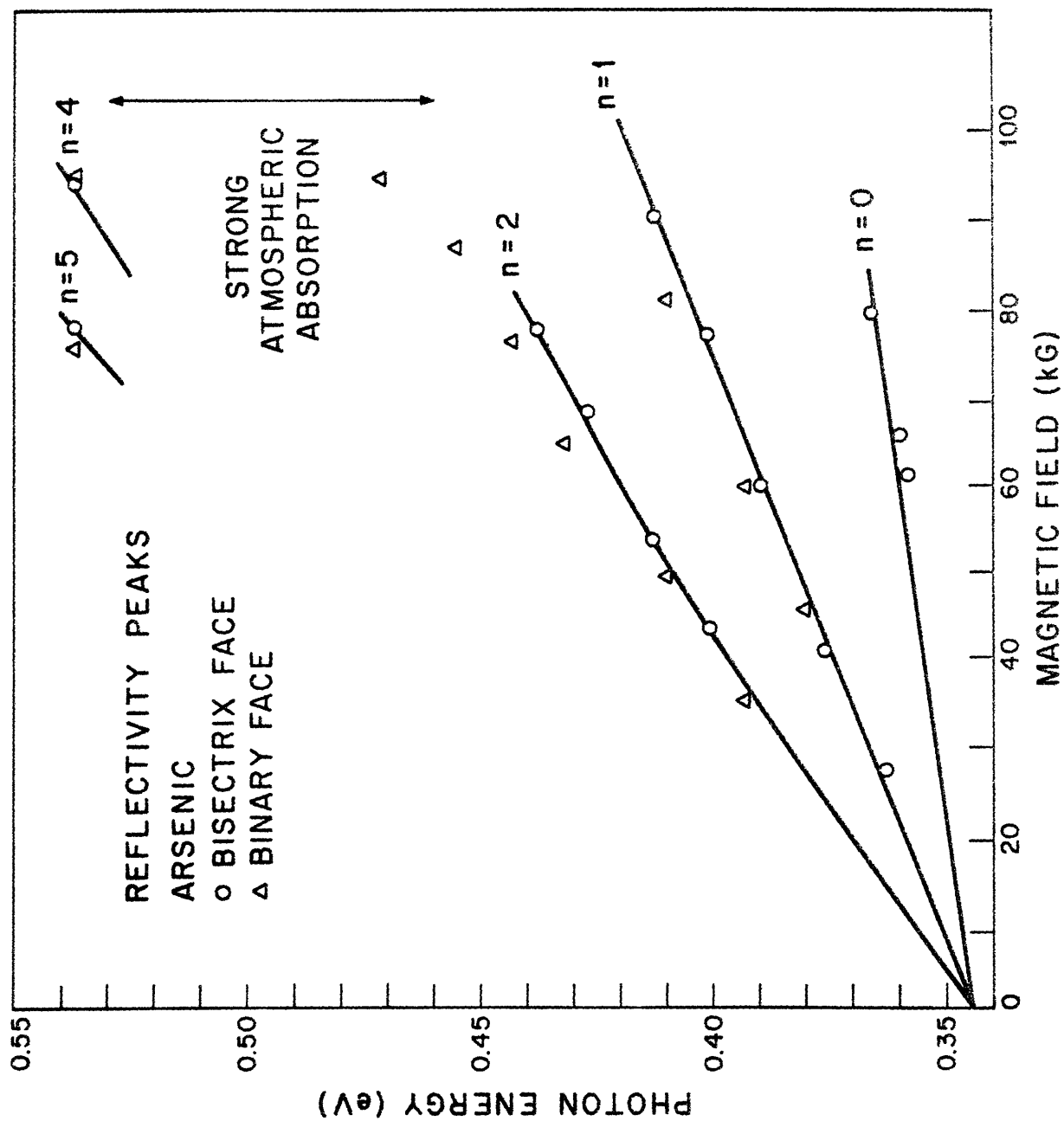


FIGURE 29

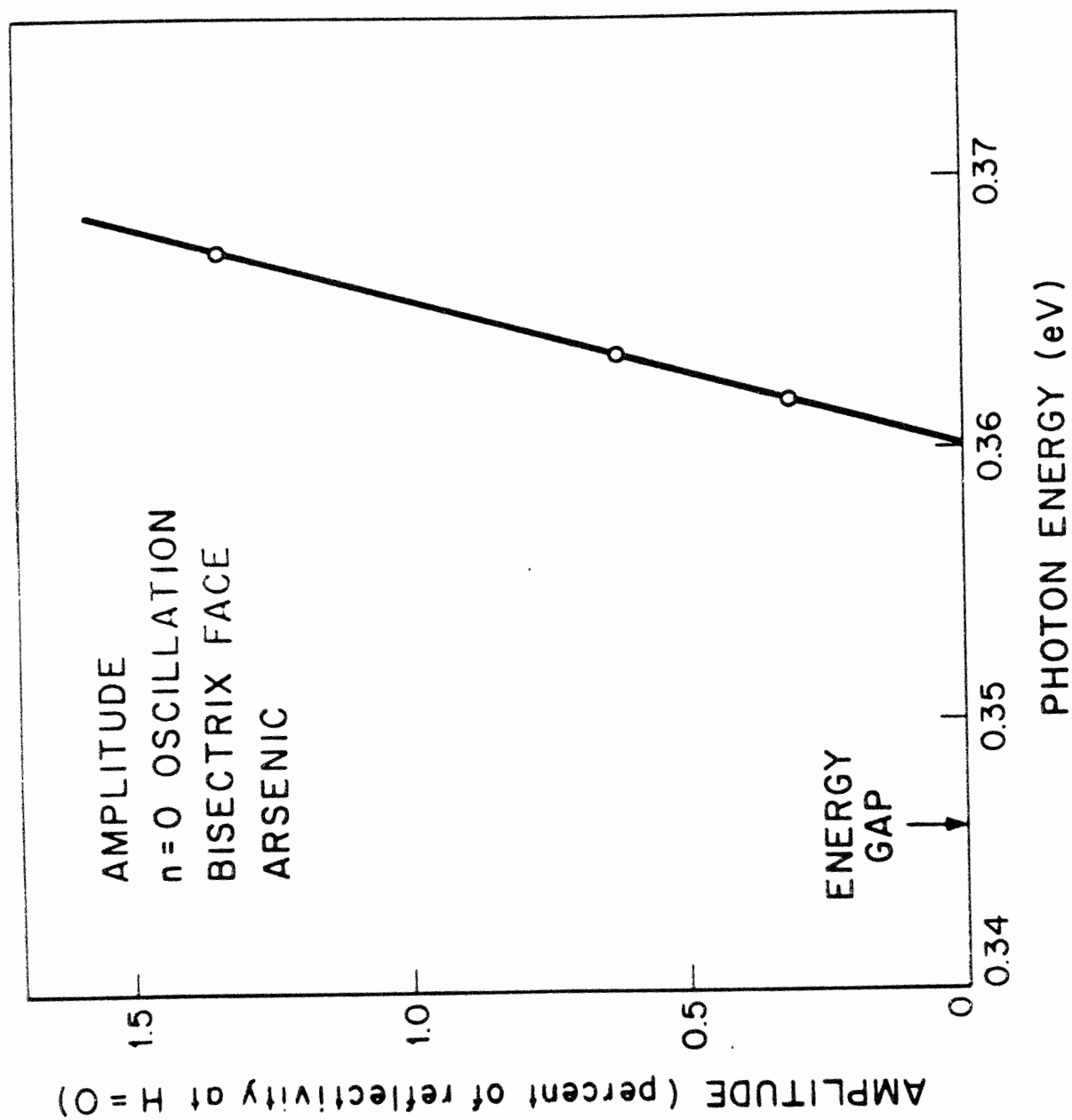


FIGURE 30

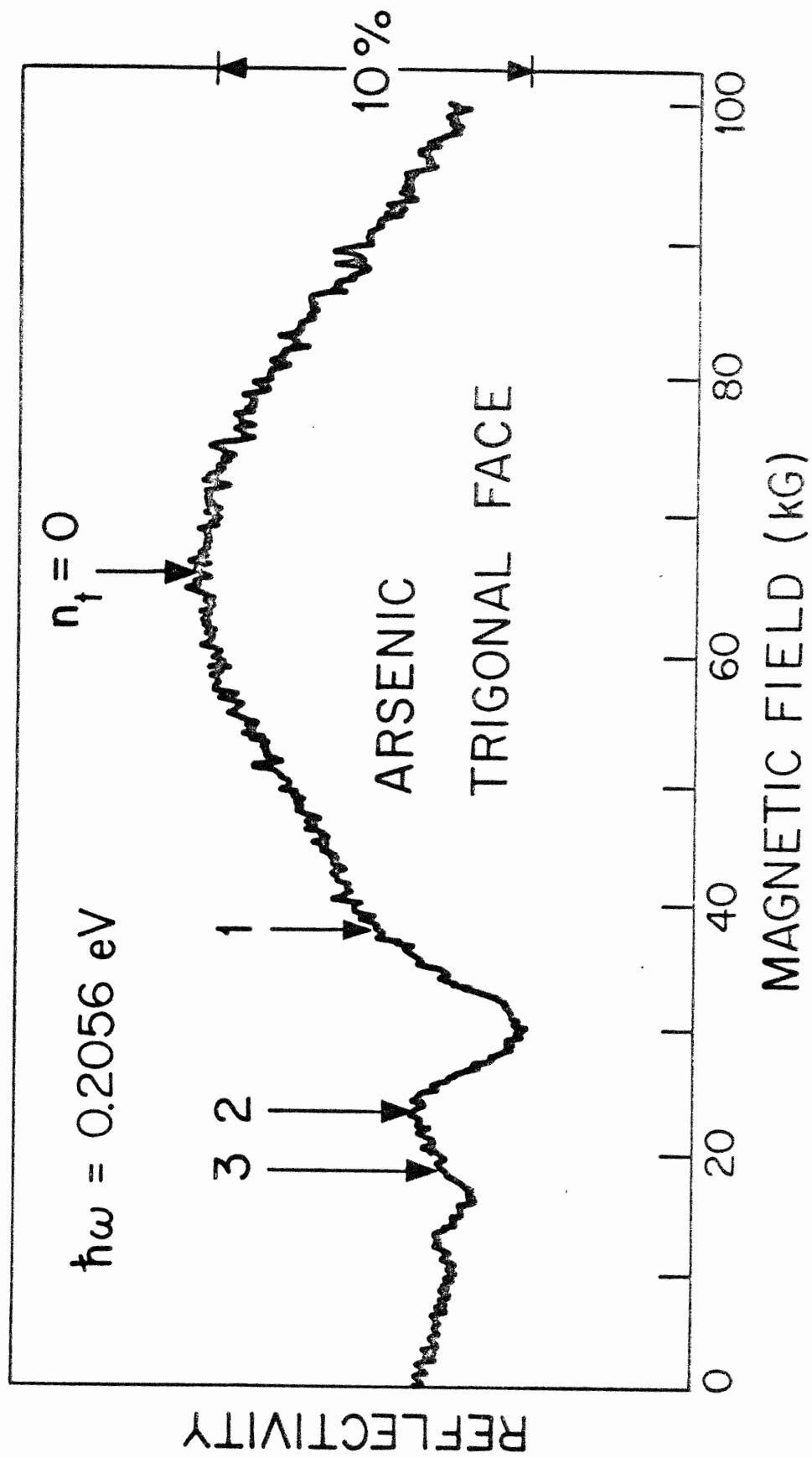


FIGURE 31a

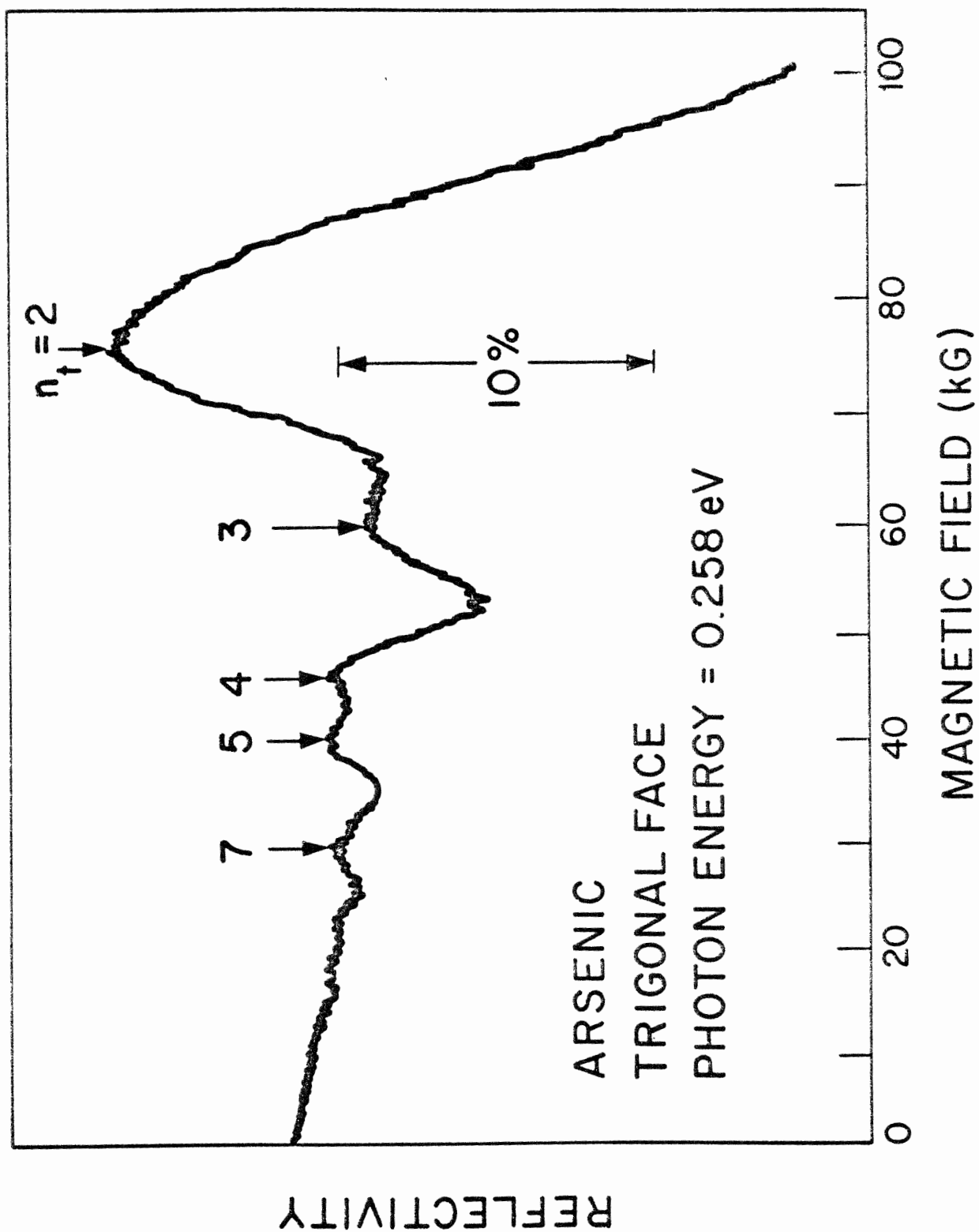


FIGURE 31b

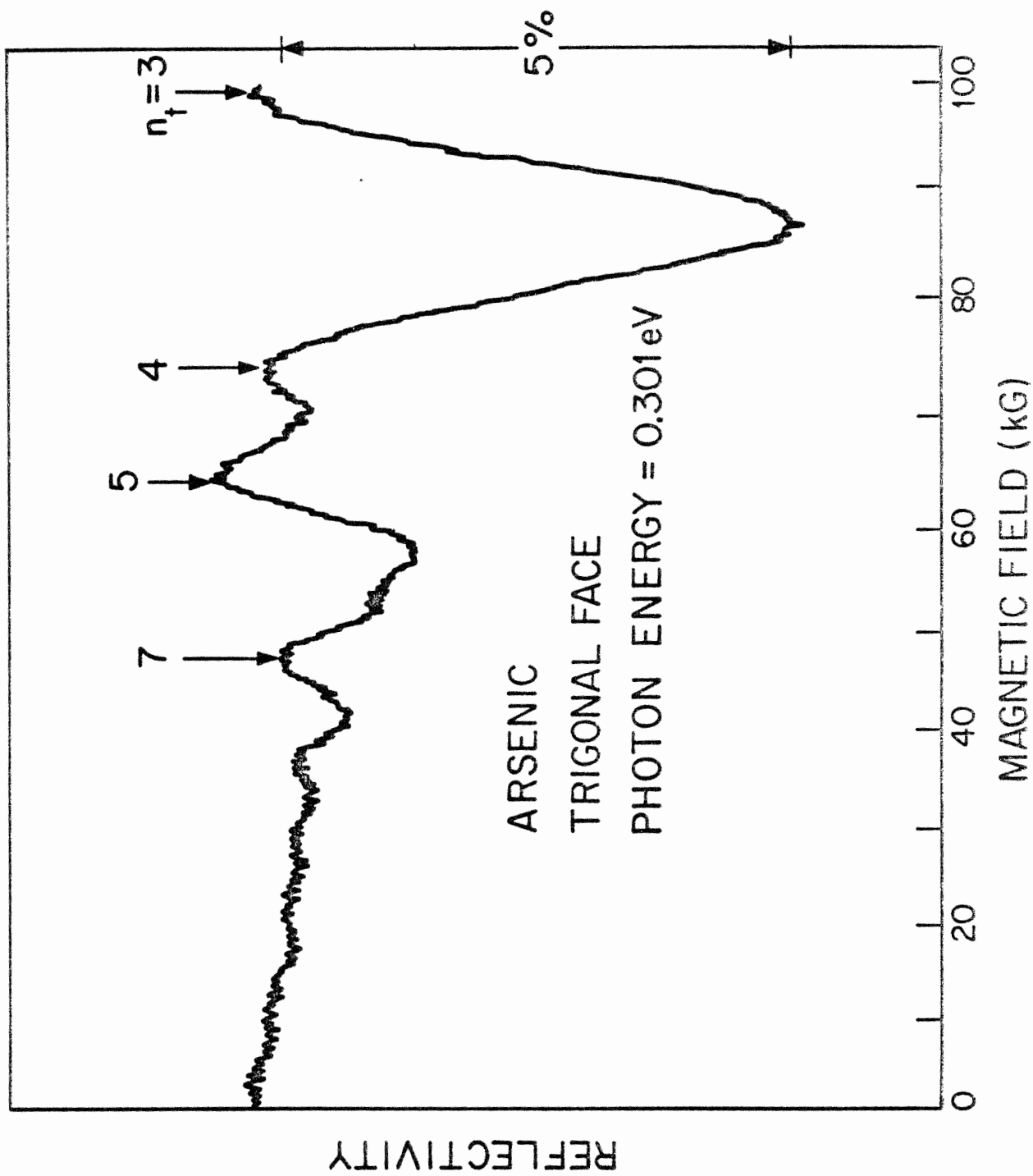


FIGURE 31c

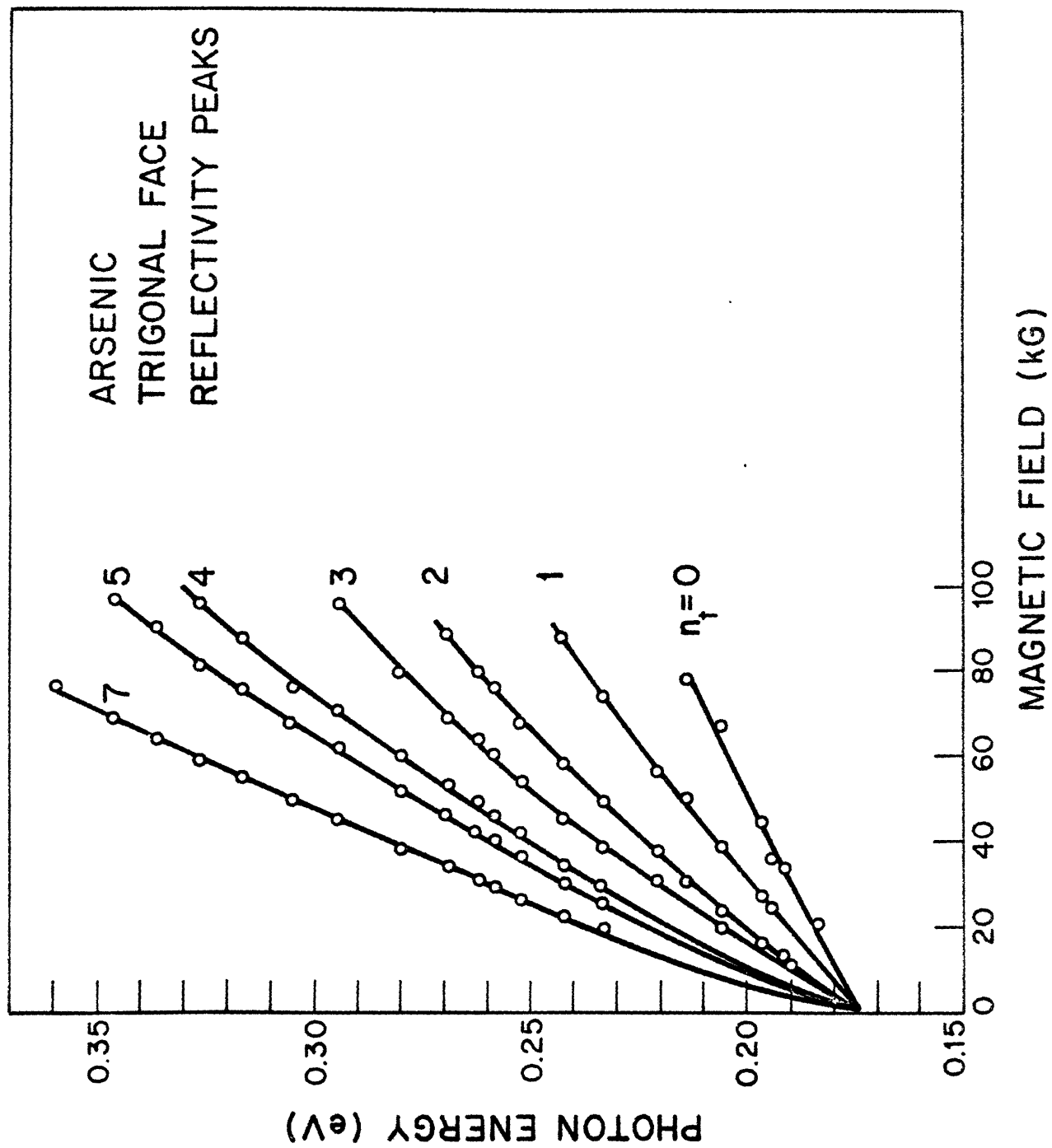


FIGURE 32

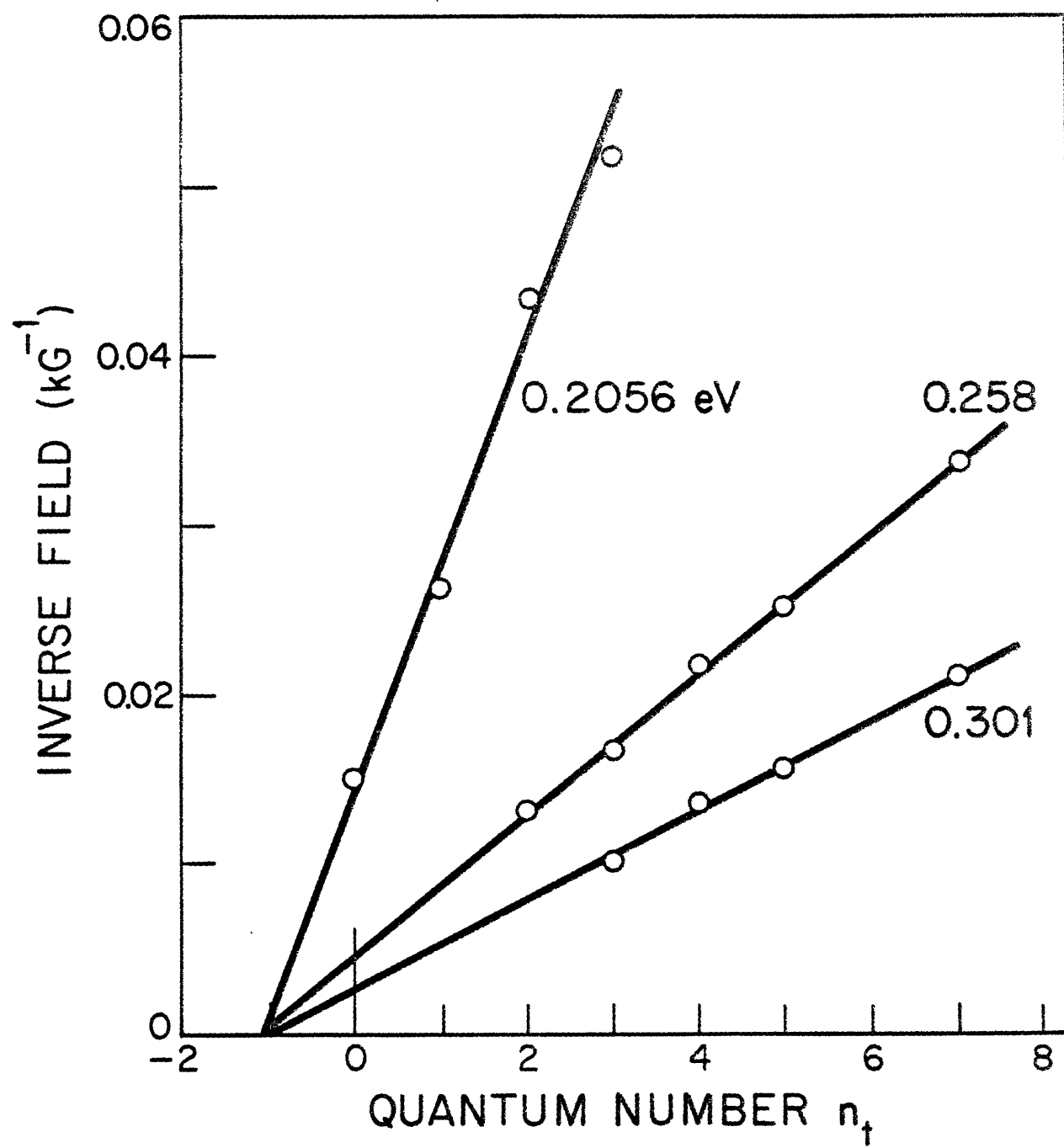


FIGURE 33

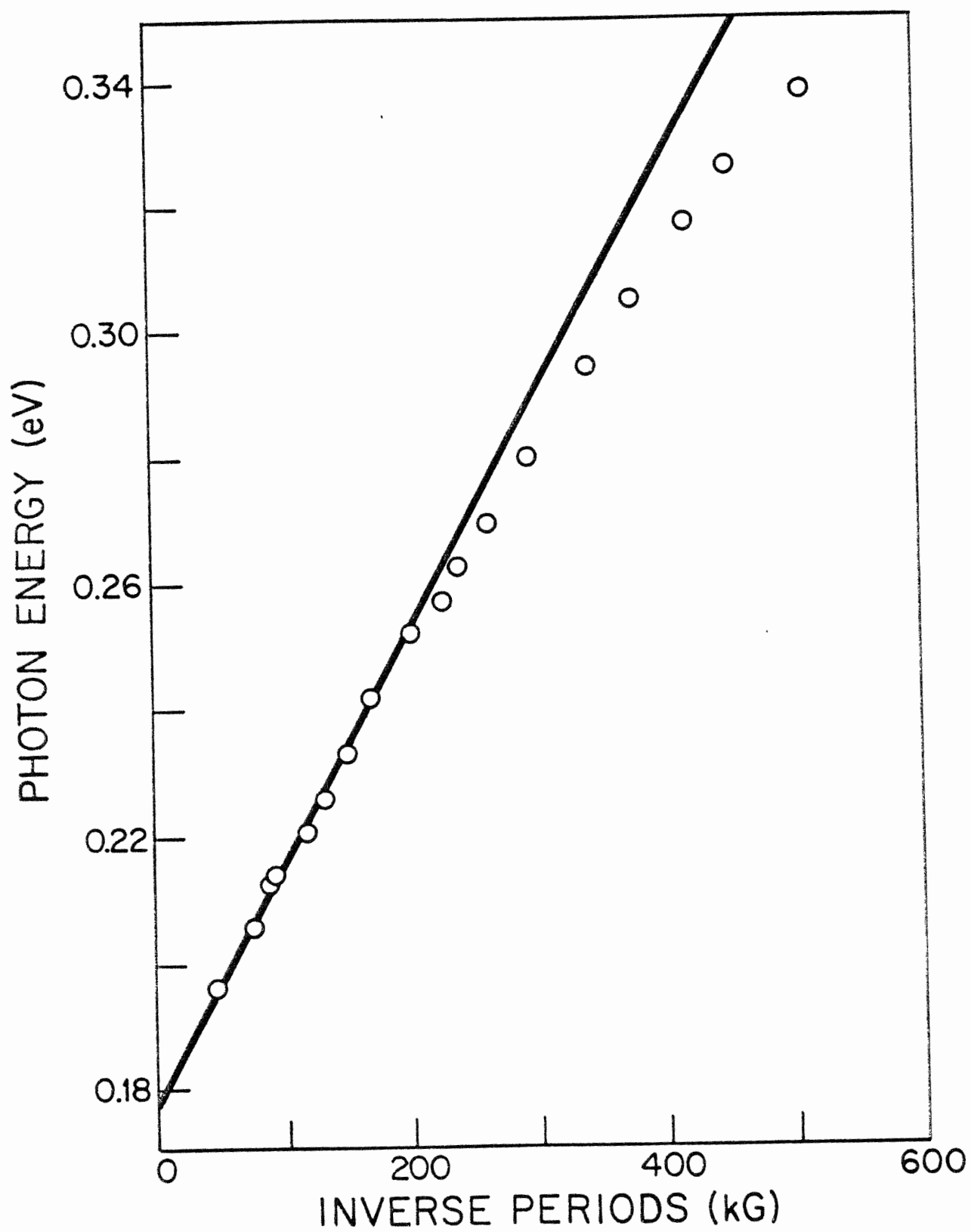


FIGURE 34

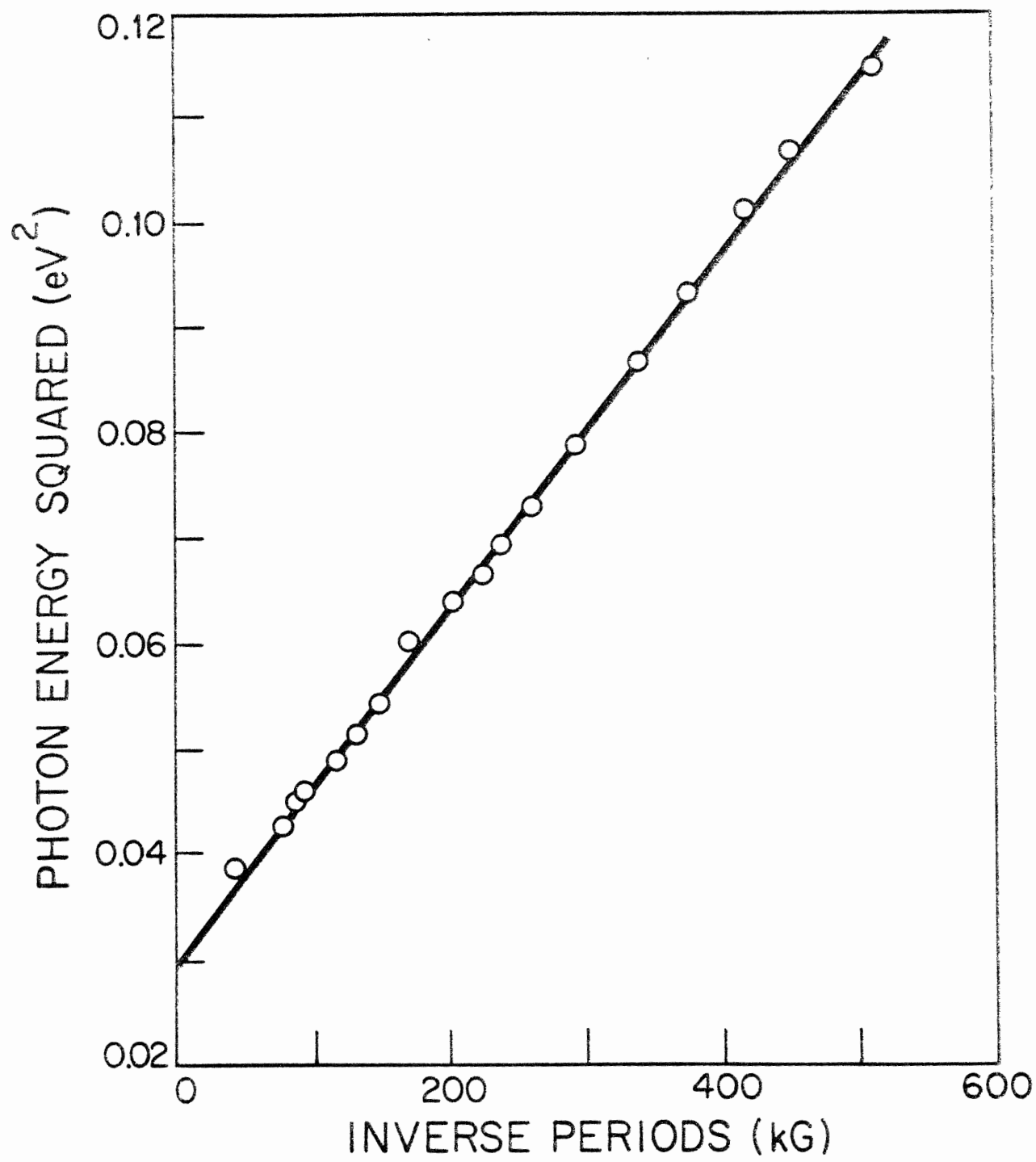


FIGURE 35

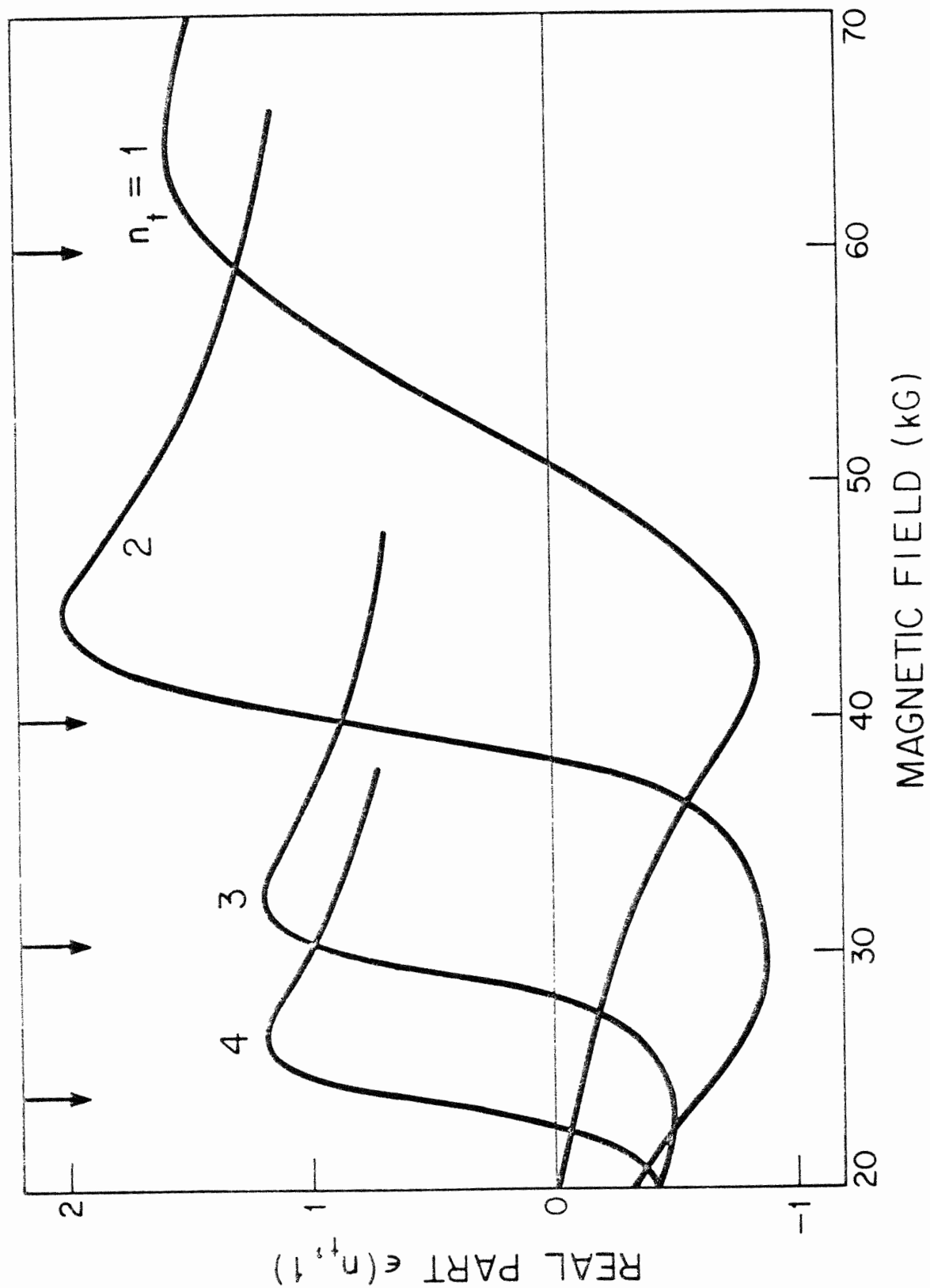


FIGURE 36

TABLE I

	MALTZ	BML	SBR	eV
$\beta^* E_g$	.011	.015	.0153	
TRIGONAL	.00125		.00082	} $\frac{eV}{kG}$
BINARY	.00747	.00472	.00550	
BISECTRIX			.000416	
	.00844	.00547	.00636	
	.00424	.00255	.00318	
$\beta^* E_g$				
TRIGONAL	14		13	} $\frac{eV^2}{kG} \times 10^{-6}$
BINARY	82	71	84	
BISECTRIX			6.2	
	93	82	97	
	47	38	49	

TABLE II

$E_g = .011\text{eV}$	$\hbar/\tau_F = .001\text{eV}$	$\epsilon_{11} = 29$
$\hat{\epsilon}_{O.L.} = .044\text{eV}$	$\hbar/\tau_c = .002\text{eV}$	$\epsilon_1 = 72$
$\hat{\epsilon}_u = .2\text{eV}$	$\hbar/\tau_h = .0008\text{eV}$	Polarization = 30%

$$\vec{m}^* = \begin{pmatrix} .00088 & 0 & 0 \\ 0 & .233 & .0263 \\ 0 & .0263 & .00509 \end{pmatrix}$$

 $v(\text{mev/kG})$

	Light ellipsoid	Heavy ellipsoid
$H \text{bin}$	-.0758	-.0116
$H \text{bis}$	-.0441	-.0218
$H \text{Trig}$	.0365	.0365

$$\vec{m}_1 = \begin{pmatrix} .064 & 0 & 0 \\ 0 & .064 & 0 \\ 0 & 0 & .69 \end{pmatrix}$$

$$\vec{m}_s = \begin{pmatrix} .033 & 0 & 0 \\ 0 & .033 & 0 \\ 0 & 0 & 200 \end{pmatrix}$$

TABLE IIIa

 γ CarriersReciprocal Effective Mass Tensor^(a)

$$\vec{\alpha} = - \begin{pmatrix} 23.9 & 0 & 0 \\ 0 & 59.5 & 10.3 \\ 0 & 10.3 & 1.22 \end{pmatrix}$$

Fermi Level ^(b)		= .011eV
Area, ^(c) H trig, Priestley et al ^(b)		= 6.9×10^{-5}
" " Lin and Falicov ^(d,e)		= 6.9×10^{-5}
Tilt angle, Priestley et al ^(b)		= -10°
" " Lin and Falicov ^(d)		= -11°
m^* , H trig Priestley et al ^(b)		= .028
" " present work		= .0269

- a) derived from orientation dependence of DHVA periods measured by Priestley et al,⁽⁶⁾ requiring m^* for H||trig to be .028.
- b) Priestley et al, ref. 6.
- c) all areas in atomic units.
- d) Lin and Falicov, Ref. 12.
- e) Lin and Falicov⁽¹²⁾ hole Fermi level set to fit the area measured by Priestley et al⁽⁶⁾.

TABLE IIIb

 α Carriers

	Theory (d)	Experiment
Fermi Energy	.361eV	.180eV ^(b)
Carrier Density/Ellipsoid		$3.9 \times 10^{19} \text{ cm}^{-3}$ (b)
Tilt Angle (min. area)	44°	37.25° ^(b)
Area ^(c) (min. area)		3.981×10^{-3} (b)
m [*] (min. area)		.096 ^(e)

 β Carriers

	Theory (d)	Experiment
Fermi Energy	.367eV	.190eV
Carrier Density/Ellipsoid		$7.07 \times 10^{19} \text{ cm}^{-3}$ (b)
Tilt Angle (min. area)	80°	86.4° ^(b)
Area ^(c) (min. area)	.0055	.005695 ^(b,f)
m [*] (min. area)		.127 ^(e)
Area ^(c) , H bin, Principal Ellipsoid	.016	.02 ^(b)
m [*] , H bin, Principal Ellipsoid		.404 ^(e)
m [*] , H bin, Non-Principal Ellipsoid	.11	.150 ^(e)
Area ^(c) , H trig.	.018	.021 ^(b)
m [*] , H trig.		.361 ^(e)
m [*] , H bis, Non-Principal Ellipsoid		.130 ^(e)

e) Chung-Sen In, see ref. 7.

f) Lin and Falicov⁽¹²⁾ electron Fermi level set to fit hte area measured by Priestley, et al.⁽⁶⁾

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BIOGRAPHICAL NOTE

The candidate was the firstborn son of Ann and Louis Maltz, and was brought into the world on January 6, 1941 in the borough of the Bronx, New York. He attended public school at P.S. 76 in the Bronx, and secondary school at the Bronx High School of Science, from which he graduated in June, 1958. He received his B.S.E.E. from the Rensselaer Polytechnic Institute in Troy, New York in June, 1962, and began his graduate studies at M.I.T. the following fall. His M.S. was received in September, 1963 in the Electrical Engineering Department, and his Ph.D. will be received in June, 1968 from the same Department.