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The Effective g-factor of Holes in Bismuth*

I. Introduction

Measurements have been made of the Shubnikov-de Haas effect in bismuth at 1.5°K and fields up to 88 kG. The effect consists of oscillations in the resistance as a function of magnetic field. The oscillations result from the quantization of the transverse energy of the carriers in a magnetic field. From the positions of the oscillations, one can obtain information concerning the band structure. In the present investigation, we have obtained values of the g-factors for holes in bismuth and have determined the variation of Fermi energy as a function of magnetic field. First an outline of the theory will be presented and then the results.

II. Theory

The important quantity in determining the oscillations in resistance is the density of states of the carriers. When an electron scatters, the scattering probability will depend upon the density of final states and hence if the density of states is an oscillatory function of the field strength, H, then the scattering time τ will exhibit oscillatory behavior as well.

At 0°K, the number of electrons below an energy E for a single isotropic band is[1]

$$N(E) = \frac{2^{\frac{3}{2}}eH}{h^2c}\, m^{\frac{1}{2}} \sum_{n,s}^{\mathcal{E}<E} [E - \mathcal{E}(n, s)]^{\frac{1}{2}}, \qquad (1)$$

where

$$\mathcal{E}(n, s) = (n + \tfrac{1}{2})h\omega_c + \tfrac{1}{2}sh\omega_s,$$

$\omega_c = eH/mc$ is the cyclotron frequency and $\omega_s = eH/m_sc$ is the spin frequency. The sum is over orbital quantum number $n\,(=0, 1, 2, \cdots)$ and spin quantum number $s\,(= \pm 1)$ and m is the effective mass. The spin mass, m_s, is defined by $m_s = 2m/g$, where g is the effective g-factor.[2] The density of states is found by differentiating (1) with respect to energy and evaluating the result at the Fermi energy E_F.

Applying this result to bismuth is slightly more complicated. Bismuth is a semimetal with a Fermi surface consisting of three tilted electron ellipsoids and one hole ellipsoid of revolution. The two band model[3] was assumed for the electron band and the spin mass tensors were assumed to have the same form as the effective mass tensors. The electron and hole bands overlap by an energy E_0, and the electron band is separated from the next lower band by an energy gap, E_G, which is an important parameter in the two band model. The Fermi energy at a given magnetic field is found by setting the number of holes, N_h, equal to the total number of electrons:

$$N_h = \sum_{i=1}^{3} N_i^e$$

where N_i^e is the number of carriers in one of the electron ellipsoids. Since the N's are a function of field, the Fermi energy will also be a function of field. The density of states is then evaluated at the Fermi energy as a function of field and the band parameters varied so that maxima in the density of states correspond to the experimentally found maxima in the resistance. A digital computer was necessary for this calculation.

III. Results

The measurements were made by inserting the sample in an impedance bridge, balancing at zero magnetic field and then plotting the unbalance of the bridge as a function of field. A photograph of such a recorder plot is shown in Figure 1 for a few orientations of magnetic field in the bisectrix-trigonal plane. For the field along the bisectrix axis (90° in Figure 1), the last electron level passes through the Fermi surface at 25 kG. The oscillations at higher fields we attribute to holes. As the magnetic field is rotated toward the trigonal axis, it is seen in Figure 1 that the hole oscillations are split by spin. Two of the levels, $n = 5$, $s = \pm 1$, have been indicated by lines drawn on the recorder chart. A plot of the positions of the hole oscillations vs quantum number n is shown in Figure 2

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* A summary.

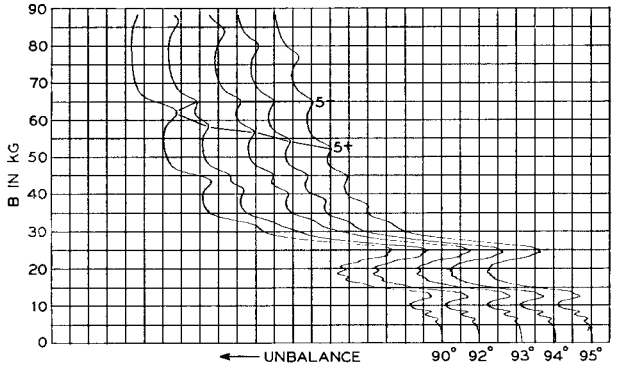

Figure 1 **A plot of impedance bridge unbalance vs magnetic field for field direction in the bisectrix-trigonal plane.** *The bisectrix axis is at 90°.*

for **H** parallel to the bisectrix axis. If the Fermi level were a constant, the plot would be a straight line and this is clearly not the case. The variation in Fermi level that is necessary for the theoretical fit to the data in Figure 2 is shown in Figure 3.

Because the oscillations are not periodic in $1/H$, individual quantum levels rather than periods have been plotted as a function of magnetic field direction. Such a plot for field rotation in the bisectrix-trigonal plane is shown in Figure 4. The hole oscillations are shown by solid lines and the electron oscillations by dashed lines. A few of the levels have been labeled with their quantum numbers, e.g., the 6+ level means $n = 6$ and $s = +1$. It is seen that the spin splitting is small parallel to the bisectrix axis (Y), becomes equal to the Landau spacing about 10° away and is almost twice the orbital splitting about the trigonal axis (Z).

The Fermi surface for the holes (in zero magnetic field) is given by

$$(E_0 - E_F) = \tfrac{1}{2}\left(\frac{p_x^2 + p_y^2}{M_1} + \frac{p_z^2}{M_3}\right), \qquad (2)$$

where **p** is the momentum and M_i are the effective mass components. The effective mass parameters, spin mass

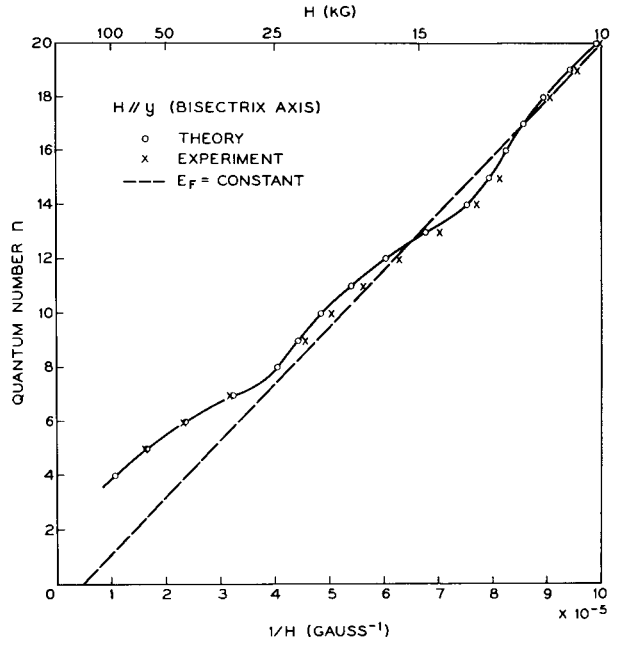

Figure 2 **Quantum number n vs inverse magnetic field. The solid line is drawn through the theoretical points.**

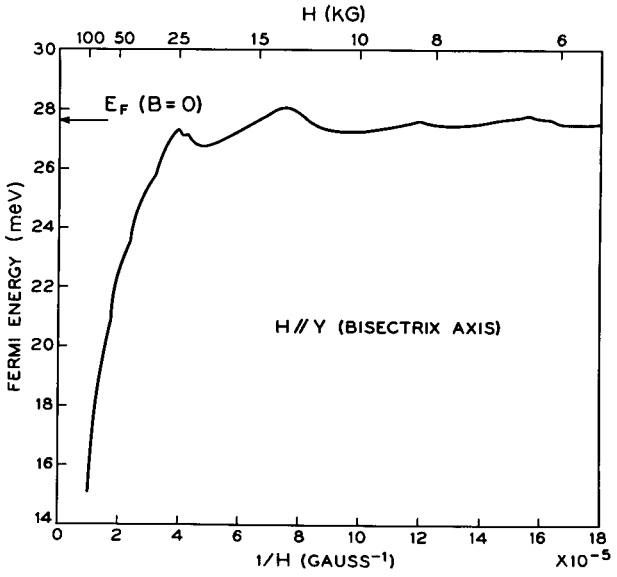

Figure 3 **Fermi level vs inverse magnetic field for H parallel to the bisectrix axis.**

Table 1

Hole Masses	M_1	M_3
Orbital	0.064	0.69
Spin	0.033	200

$E_0 = 38.5$ meV. $E_g = 15.3$ meV. $E_F(B = 0) = 27.6$ meV.

parameters (see Ref. 2), and pertinent energies used in the theoretical plots to fit the data are given in Table 1. The large value of M_3 for the spin mass tensor reflects the fact that splitting could not be observed parallel to the bisectrix axis. This value could be larger without affecting the theoretical fit.

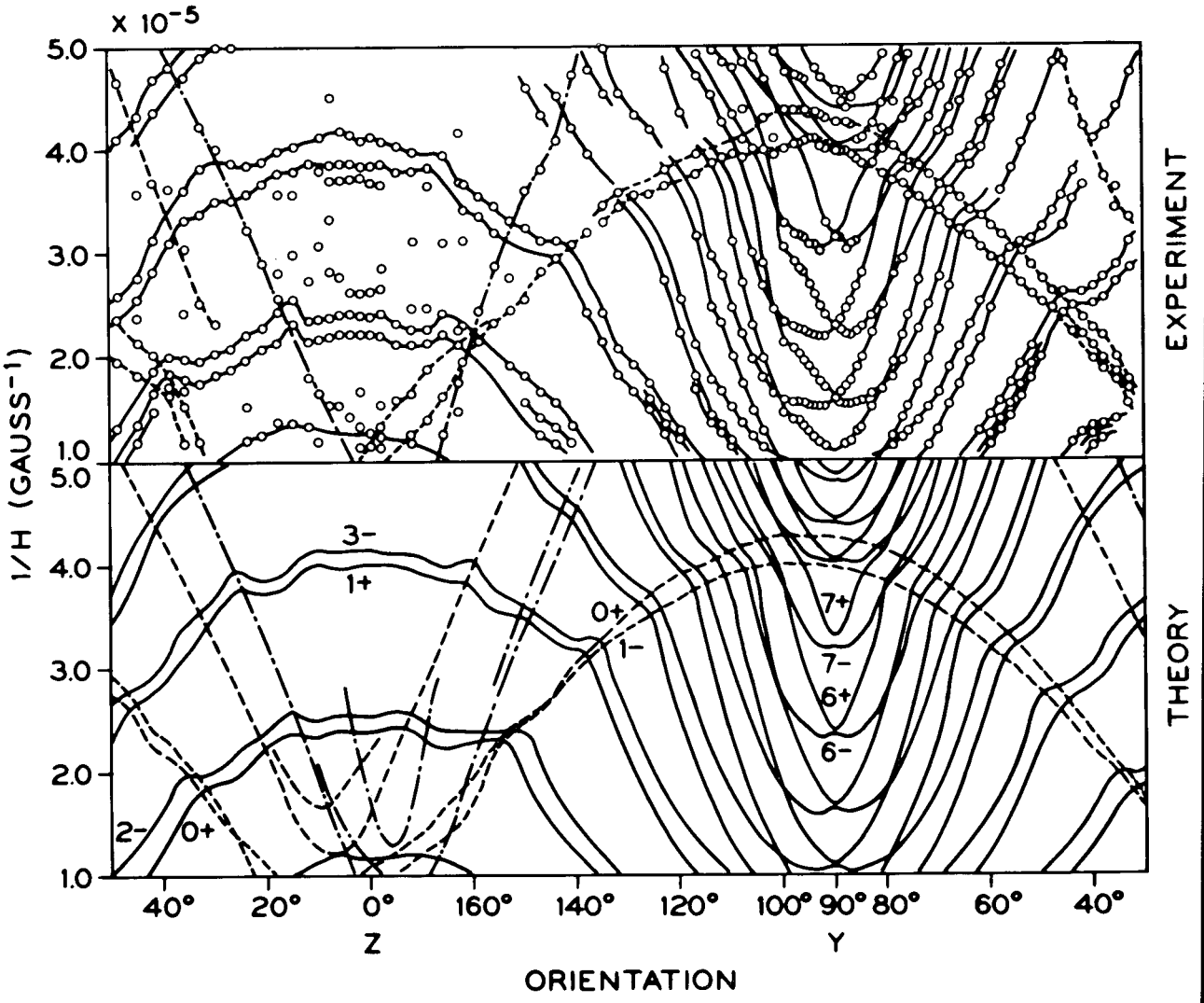

Figure 4 **Experimental and calculated plots of individual quantum levels vs magnetic field direction in the bisectrix-trigonal plane.** *Most electron levels about the trigonal (Z) axis were omitted because the closeness of the levels did not permit an unambiguous level assignment.*

The electron effective mass parameters used are essentially those found from microwave resonance experiments.[4] Spin splitting of electron oscillations has been seen and a tentative interpretation shows a spin splitting smaller than the Landau spacing for heavy mass directions and slightly larger than the Landau spacing for light mass directions.

IV. Discussion

The principal new results of the investigation have been the observation of spin splitting of the hole band and an exact density of states calculation which exhibits the observed variation in Fermi energy at high fields. The model chosen for the effective spin mass tensor was cigar shaped and a good fit to the data was achieved. Two other models were tried, a pancake shape and a scheme where the g-factor is positive along one axis and negative along the other, but a fit was not to be found.

References

1. R. E. Peierls, *Quantum Theory of Solids*, Oxford University Press, London, 1955, p. 147.
2. M. H. Cohen and E. I. Blount, *Phil. Mag.* 5, 115 (1960).
3. B. Lax, J. G. Mavroides, H. J. Zeiger, and R. J. Keyes, *Phys. Rev. Letters* 5, 241 (1960).
4. G. E. Smith, L. C. Hebel and S. J. Buchsbaum, *Phys. Rev.* 129, 154 (1963).

Discussion

M. H. Cohen: Could you please recall briefly to our minds how these values of gap, overlap and Fermi energy compare with previous determinations?

G. E. Smith: Brown, Mavroides and Lax [*Phys. Rev.* **129**, 2055 (1963)] found $E_g = 15$ meV and $E_F = 25$ meV (for electrons). We use 15.3 and 27.6 meV. I have a feeling that the difference may be due just to differences in purity of the samples.

Dale Brown: How sensitive is your data to the value of the optical band gap which determines the amount of nonparabolicity? Can you distinguish, for example, between the values 40 meV and 15 meV that have been reported on and off in the literature?

Smith: Not that finely. It is between 13 and 17 meV so far as our data is concerned.

Brown: You're assuming that the nonellipsoidal nonparabolic model is correct, *a priori*? Then you're trying to get the band gap by fitting the effective mass data, essentially?

Smith: Yes. The justification is that fitting the individual points in the plot which was shown, which takes into account the variation in Fermi energy, is rather sensitive to E_g; and we fit all the points within a couple of percent—or certainly within the resolution. About the trigonal axis, as I say, we're not sure; but we do feel we have in general a good fit with this model, and there appears to be no need for another.

Brown: I might point out that this value is very important for the determination of the number of electrons per ellipsoid, and one can get into trouble in the literature according as to which value of E_g you use and what value of total electron concentration you use, as far as determining the number of equivalent ellipsoids.

Smith: Yes, one criterion that we did have was that the number of electrons be equal to the number of holes and one assumes that the hole band is a parabolic band, which again may not be the right assumption. The hole oscillations do give a good value for the number of holes and this would naturally have to equal the number of electrons.

S. H. Koenig: I'd like to point out something concerning what Brown just said. You really don't have to know this gap to get the total number of carriers in the band except insofar as it determines any deviation from ellipsoidal shape at the Fermi surface, which one knows to be small (about 5%, say). All you really have to know is enough cross sectional areas of the Fermi surface to get the total number density. This has recently been done by R. D. Brown, who obtained all the cross sections required. His result was 0.95×10^{17} electrons per cm^3 per ellipsoid, before this 5% correction. I don't think this correction is very sensitive to a variation of the gap—even a factor of two variation.

N. Goldberg: You have the electron-spin splitting smaller than the Landau splitting in the X direction and larger than the Landau splitting in the Y direction?

Smith: No, there are three sets of electrons and one of the electron's masses, the heavy cyclotron mass, has a spin splitting smaller than the Landau splitting along the X axis and the other two have a spin splitting larger than the Landau splitting along the X axis. Along the Y axis, they are both larger.

Goldberg: Wouldn't you expect the impedance to go in different directions depending on whether the spin splitting was larger or smaller than the Landau splitting?

Smith: If you're talking about the case where the spin splitting would be smaller for both the electrons and holes, then one would expect the bottoms of the bands to uncross and bismuth then to become a semiconductor. But for bismuth there is no orientation for which this is the case; there is always some splitting which will maintain an overlap between the two bands.

S. J. Buchsbaum: Can some expert compare the g values just reported with the spin masses which were reported earlier and find out if they fit?

Smith: We have agreed privately that they did fit.