tion $\sin^2\delta=\delta^2$. Thus, very directly for this term, we obtain the form (18), in which the interaction between different times is given not by the singular function $1/(x_1-x_2)^2$ but by $G_0{}^2(x_1-x_2)$, which has the singular behavior cutoff at $x_1-x_2=\tau$. To within this approximation, we can, thus, show that a cutoff at time τ_0 appears again. Higher-order terms are about as straightforward as any Feynman diagram of the same order, and are unlikely to give us drastically different results.

Thus, in at least three distinct cases, we can work out the mathematics of the cutoff precisely. None of the results are identical in detail, but all behave in very similar fashion. Further effort in elucidating the numerical nature of the cutoff is physically unwarranted, since in fact we are seldom or never confronted with known form factors and band structures; it is only the Fermi-surface-dependent features of the problem which are of any real physical interest.

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Band Structure of the Holes in Bismuth

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A study of the band structure for the holes in Bi has been by the magnetoacoustic effect in a Sn-doped Bi sample. The existence of a singular point of the saddle type is confirmed and a new pocket of holes is found. The analysis of the experimental results supports the Golin band calculation in Bi.

1. INTRODUCTION

In a previous paper,[1] the existence of a singular point of the saddle type for the holes in bismuth was postulated to explain some experimental results. The main feature of the experiments was the disappearance of the oscillations of the ultrasound absorption coefficient as a function of the magnetic field strength when the hole Fermi surface was investigated.

To confirm and clarify the hole-band structure of bismuth a new set of measurements has been carried out in a sample of Sn-doped Bi, with a concentration of impurity of 4.5×10^{18} cm^{-3}, in order to have only hole carriers.[2] The interpretation of the experimental results, in particular the location of the double-conic point along the binary direction, is consistent with the Golin band-structure calculation[3] of bismuth.

The present work is concerned with measurements, by means of the magnetoacoustic effect, of the cross-sectional area S of the Fermi surface and of the phase factor γ of the semiclassical quantization rule, $S(\epsilon_F,k_H)=(n+\gamma)(2\pi eH/c\hbar)$, for various magnetic-field and sound-wave vector directions.

In Sec. 2 the theoretical background is outlined; in Sec. 3 the experimental results are presented; in Sec. 4 a dispersion law and a model of the hole Fermi surface are deduced from the experimental measurements.

[1] M. Giura, R. Marcon, T. Papa, and F. Wanderlingh, Phys. Rev. **179**, 645 (1969).
[2] J. M. Noothoven Van Goor, Phys. Letters **21**, 603 (1966).
[3] S. Golin, Phys. Rev. **166**, 643 (1968).

2. THEORY

In this section some particular aspects of the existence of a singular point of saddle type in the $\mathbf{k}$ space are analyzed.

Around a saddle point the dispersion law of the carriers can be approximated as follows:

$$\epsilon=\epsilon_0+\alpha_1k_1{}^2+\alpha_2k_2{}^2+\alpha_3k_3{}^2\,, \tag{1}$$

with the coefficients α_1, α_3 having sign opposite to α_2 and choosing k_1, k_2, k_3 as the bisector, binary, and trigonal axis, respectively.

In this case one of the authors[4] has shown, with semiclassical arguments, that the relation

$$S(\epsilon,k)=2\pi(eH/c\hbar)(n+\gamma) \tag{2}$$

is still valid and γ assumes the value of $\frac{3}{4}$. This result has been obtained when the magnetic field is along the k_3 axis and in relation with all the values of the momentum k_3 that do not lead in the $\mathbf{k}$ space to self-intersecting orbits for carriers. In the case of self-intersecting orbits, the semiclassical arguments, in fact, are not valid.[5]

The value $\gamma=\frac{3}{4}$ follows from the structure of the differential equation derived from Eq. (1) by means of the Luttinger and Kohn[6] procedure in the presence of

[4] M. Giura, Phil. Mag. (to be published).
[5] M. Giura and F. Wanderlingh, Phys. Rev. Letters **20**, 445 (1968).
[6] J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).

an uniform magnetic field. Moreover, the structure of the differential equation depends in an essential way on the direction of the magnetic field.

As a consequence a cone exists that divides the **k** space into two parts with the following results: For directions of the magnetic field outside the cone the value of γ is $\frac{3}{4}$, while inside the cone γ assumes the value of $\frac{1}{2}$.

To show this, the procedure of Baldareschi and Bassani[7] is followed.

Starting from a dispersion law as in Eq. (1) with $\alpha_1=\alpha_x h^2$, $\alpha_2=\alpha_z h^2$, etc., and choosing a gauge where the vector potential is defined by

$$\mathbf{A}=\tfrac{1}{2}\mathbf{H}\times\mathbf{r}+\tfrac{1}{2}\,\mathrm{grad}[H_y xz+H_z zy-H_x yz], \qquad (3)$$

Baldareschi and Bassani are able to write the Hamiltonian in the form

$$\mathcal{H}=(\alpha/\beta)p^2+(e^2/c^2)\beta q^2+(\alpha_x\alpha_y\alpha_z/\alpha)S^2, \qquad (4)$$

where

$$\alpha=\alpha_x\alpha_y H_z^2+\alpha_z\alpha_x H_y^2+\alpha_y\alpha_z H_x^2$$

and

$$\beta=\alpha_z H_x^2+\alpha_x H_z^2.$$

$S=\mathbf{H}\cdot\mathbf{p}-(e/c)H_z H_y x$ is a constant of motion and p and q are two new canonically conjugate variables.

When $\alpha>0$ the Hamiltonian (4) is that of a harmonic oscillator and a semiclassical argument gives the value $\frac{1}{2}$ for γ.

When $\alpha<0$, Eq. (3), of the same type as that of the work cited above[4] and valid for a particular direction of the magnetic field, leads to the value of $\frac{3}{4}$ for γ.

The condition for $\alpha=0$ gives an elliptical cone in the **k** space, as in Fig. 1, with the angle θ_1 and θ_3 related to the α_1, α_2, α_3 coefficients by

$$\tan\theta_1=(-\alpha_1/\alpha_2)^{1/2},\quad \tan\theta_3=(-\alpha_3/\alpha_2)^{1/2}. \qquad (5)$$

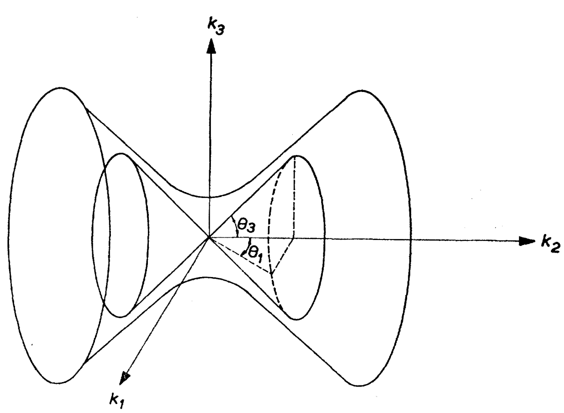

FIG. 1. Cone in the **k** space dividing the two regions for which γ assumes the values $\frac{3}{4}$ and $\frac{1}{2}$.

[7] A. Baldareschi and F. Bassani, Phys. Rev. Letters **19**, 66 (1967).

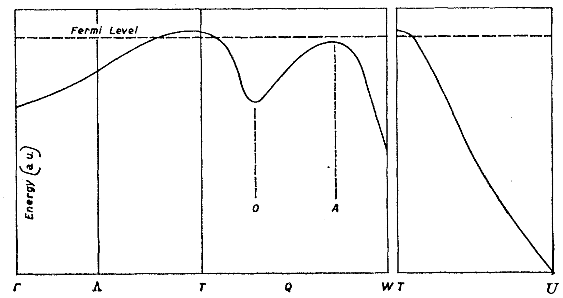

FIG. 2. Golin band structure for the holes near the Fermi level.

A measurement, then, of γ as function of the angle between the magnetic-field direction and the crystallographic axes supplys a test of the theory and a determination of the angles θ_1 and θ_3, as shown in Sec. 3.

The existence along the binary direction (k_2 direction in our reference system) of the singular-point double conic is consistent with the Golin[3] calculation as well as with the existence of a new set of carriers of a hole type in the Sn-doped samples.

The results of the Golin band calculations concerning the holes are shown in Fig. 2, from which it is possible to clearly understand that along the binary direction *TW* there can exist either a singular point of the postulated type or a new pocket of holes.

3. EXPERIMENTAL RESULTS

The measurements have been performed at Helium temperature on a sample of Sn-doped bismuth with a Sn impurity concentration of 4.5×10^{18} cm^{-3} so as to have *only* hole type of carriers.[2]

The measurements performed are essentially of two kinds:

(a) Measurements of the cross-sectional area of the Fermi surface orthogonal to the magnetic-field direction with the period of the oscillations of the acoustic-absorption coefficient as function of the magnetic-field strength.

(b) Measurements of the phase factor γ by the intersection of the straight line obtained by plotting the inverse of the magnetic field at the maxima of absorption coefficient as function of the integer Landau number.

The measurements of the (a) type are of the type previously performed by many authors[8–11] and the experimental setup is described in a previous paper.[12]

Various sets of cross-sectional area measurements

[8] P. Korolyuk and T. A. Prushckak, Zh. Eksperim. i Teor. Fiz. **41**, 1689 (1968) [English transl.: Soviet Phys.—JETP **14**, 1201 (1962)].
[9] Y. Shapiro and B. Lax, Phys. Rev. Letters **12**, 166 (1964).
[10] A. M. Toxen and S. Tansal, Phys. Rev. **137**, A211 (1965).
[11] S. Mase, Y. Fuimori and H. Mari, J. Phys. Soc. Japan **21**, 1744 (1966).
[12] M. Giura, R. Marcon, T. Papa, and F. Wanderlingh, Nuovo Cimento **51B**, 150 (1967).

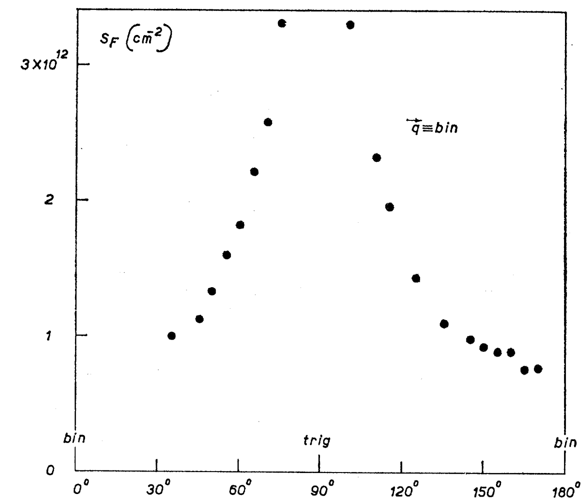

FIG. 3. Cross-sectional area for the magnetic-field directions in the trigonal-binary plane.

have been performed under the following physical situations:

(I) Ultrasound along the binary axis and the magnetic-field direction in the trigonal-binary plane (Fig. 3).

(II) Ultrasound along binary axis and the magnetic-field direction in the binary-bisector plane (Fig. 4).

The evaluation of the phase factor has been performed by assuming the hypothesis of the existence of a large spin-splitting factor, that is, the cyclotron mass equal to the spin mass. In this case, Eq. (2) for $\epsilon=\epsilon_F$, becomes

$$S(\epsilon_F\pm\tfrac{1}{2}g\mu H,\, k_H)=2\pi(eH/hc)(n+\gamma)\,, \qquad (6)$$

with $\mu=eh/2m_0c$. To a first-order approximation in

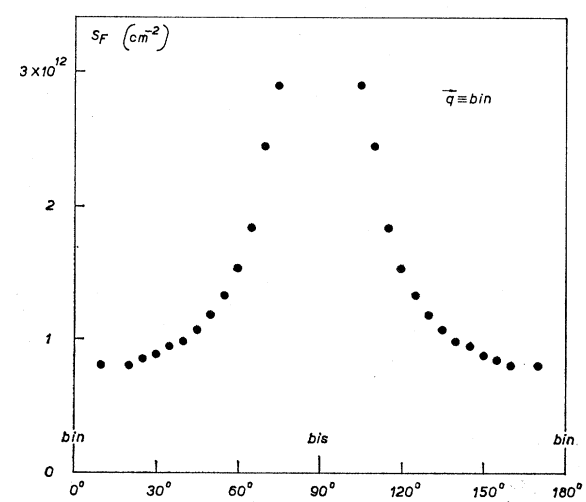

FIG. 4. Cross-sectional area for the magnetic-field directions in the binary-bisector plane.

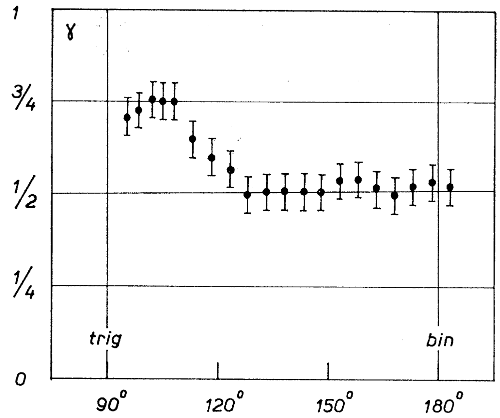

FIG. 5. γ values for H directions in the trigonal-binary plane.

$g\mu H$, that is, when $\epsilon_F\gg\frac{1}{2}g\mu H$ or $n>1$, Eq. (6) becomes

$$S(\epsilon_F,k_H)=(2\pi eH/ch)(n+\gamma)\pm(\delta S/\delta\epsilon)_{\epsilon_F}\tfrac{1}{2}g\mu H\,. \qquad (7)$$

Introducing the spin mass as $\frac{1}{2}g=m_0/m_s$ and recalling the expression for the cyclotron mass,

$$m_c=(h^2/2\pi)(\delta S/\delta\epsilon)\,,$$

Eq. (7) becomes

$$S(\epsilon_F,k_H)=(2\pi eH/ch)(n+\gamma\pm\tfrac{1}{2}) \qquad (8)$$

if $m_s\cong m_c$.[13] In the following, the analysis of the experimental results is carried out with the assumption that $m_s=m_c$. This is consistent with the fact that the experimental values of effective-mass tensor coefficients are small [see Eq. (10)][14] and also that the experimental results of the intercept, for almost all the directions of the magnetic field, give an integer value, this for $\gamma=\frac{1}{2}$ leads to $m_s=m_c$, as first pointed out by Boyle *et al.*[15]

The values of γ obtained from the experimental results by means of the least-square-fit method are plotted in Fig. 5 for the magnetic-field directions in the plane trigonal-binary, and in Fig. 6 for the magnetic field in the plane binary-bisector.

The angle at which γ changes its value from $\frac{1}{2}$ to $\frac{3}{4}$ is the same in the two cases. The same angle has been found in planes rotated around the binary axis of 30° and 60° with respect to the binary-bisector plane.

The method for the determination of γ by means the intercept of the straight line is correct because it is possible, in the present case, to have minima at low Landau quantum numbers. The determination of

[13] It is to be noted that the hypothesis $m_s=m_c$ refers to the measurements reported in point (a) above. As is discussed further, these measurements do not refer to a hole pocket centered in the T point of the Brillouin zone for which the g-factor measurements does not in general [G. E. Smith, G. A. Baraff and J. M. Rowell, Phys. Rev. **135**, A1119 (1964); Y. Eckstein and J. B. Kettenson, *ibid.* **137**, A1777 (1965)] give $m_s\simeq m_c$ but to a new type of hole pocket (centered in the point A of Fig. 2) along the binary direction TW.

[14] M. H. Cohen and E. I. Blount, Phil. Mag. **5**, 115 (1960).

[15] W. S. Boyle, F. L. Hsu, and J. E. Kunzler, Phys. Rev. Letters **4**, 278 (1960).

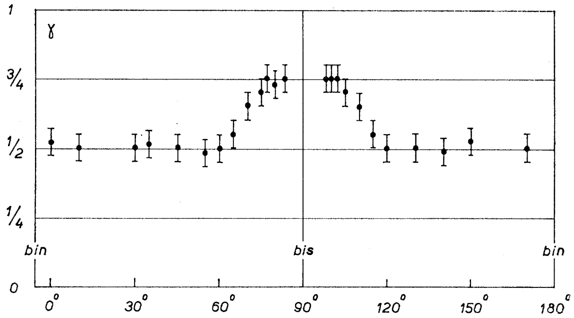

FIG. 6. γ values for H directions in the binary-bisector plane.

intercept values is carried out by finding the straight-line parameters with the least-square-fit method by means of a computer.

4. DATA ANALYSIS AND DISCUSSION

A. Saddle Points

The existence of a singular point (conic double point in Fig. 1) in the **k** space has been postulated in a previous paper to explain the disappearance of quantum-magnetoacoustic oscillations in some directions of the magnetic field.[1]

The reported measurements of the phase factor γ can be explained by the same hypothesis. Furthermore, these results give indications as to the location of the conic double point as well as information about the development coefficients of the energy around this point.

The disappearance of oscillations has been obtained when the magnetic field direction was near the trigonal axis, that is, according to the conic double-point interpretation, when the orbit-plane orthogonal to the magnetic field becomes tangent to the Fermi surface at a saddle point.[5] From these results the cone axis must belong to the bisector-binary plane. The fact that variations of the γ from the $\frac{1}{2}$ value to the $\frac{3}{4}$ value occur in the trigonal-binary and binary-bisector planes (Figs. 5 and 6), and in the planes rotated around the binary axis, allows us to say that the cone axis is the binary axis.

This is consistent with the Golin[3] calculation as reported in Fig. 2 from which is evident the existence of a double conic point O along the binary direction TW. In addition, the cone is a rotation one around the binary axis with the angle $\theta_1 = \theta_3 = (70 \pm 5)°$, that is, $\alpha_1 = \alpha_3$.

B. Hole Fermi Surface

A detailed analysis of the hole Fermi surface has been carried out by Bate and Einspruch[16] who showed

[16] R. T. Bate and N. G. Einspruch, Phys. Rev. **153**, 796 (1967).

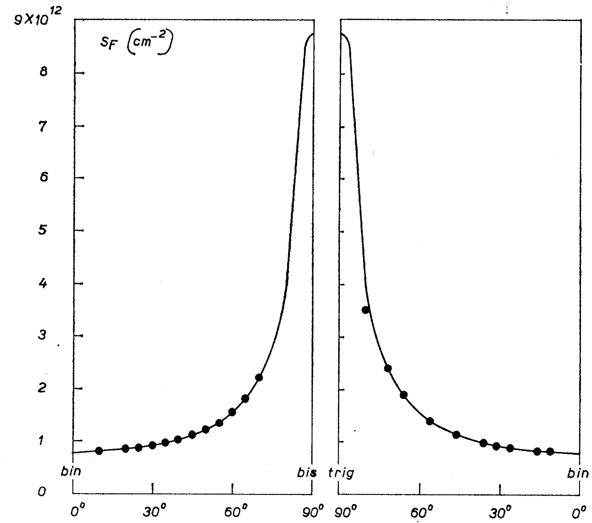

FIG. 7. Least-square fit of the cross-sectional area for an ellipsoidal model of the new holes pocket with the parameter values $(\hbar^2\beta_1/2m_0\epsilon_F) = \hbar^2\beta_3/2m_0\epsilon_F = 4\times10^{-12}$ cm², $(\hbar^2\beta_2/2m_0\epsilon_F) = 3.2\times10^{-14}$ cm². Dots refer to experimental data.

that an ellipsoidal nonparabolic model should be valid for the hole in bismuth. Their results (Fig. 4 of their work), concerning the holes show a linear increase of the Fermi hole cross-sectional area as the Sn-doping increases. The experimental results presented in this paper (Fig. 7) give a cross-sectional area smaller than that obtained at a Sn concentration of $2\times10^{18}/\text{cm}^3$, even though the Sn doping is doubled in the present case.

Further, while the cross-sectional areas for the hole at the T point have a minimum value (in the hypothesis that the band structure is not altered by doping) when the magnetic field lies in the trigonal direction, in the present case for H parallel to the trigonal axis the cross-sectional area assumes its maximum value (see Fig. 3).

This suggests the existence of a new pocket of holes centered at a point along the binary direction, that is, the present Sn concentration has been able to lower the Fermi level so that a valence band arises at the point A in Fig. 2.

The variation range of the magnetic field (up to 18 kG) in the present experiments does not permit the detection of the large cross sections of holes at the T point.

It is to be noted that the existence of this new pocket does not contradict the conclusions of Bate and Einspruch,[16] because the doping in this case is about doubled and as a consequence the lowering of the Fermi level is more than 15 meV.

As a first approximation an ellipsoidal model has been assumed for an interpretation of experimental data as

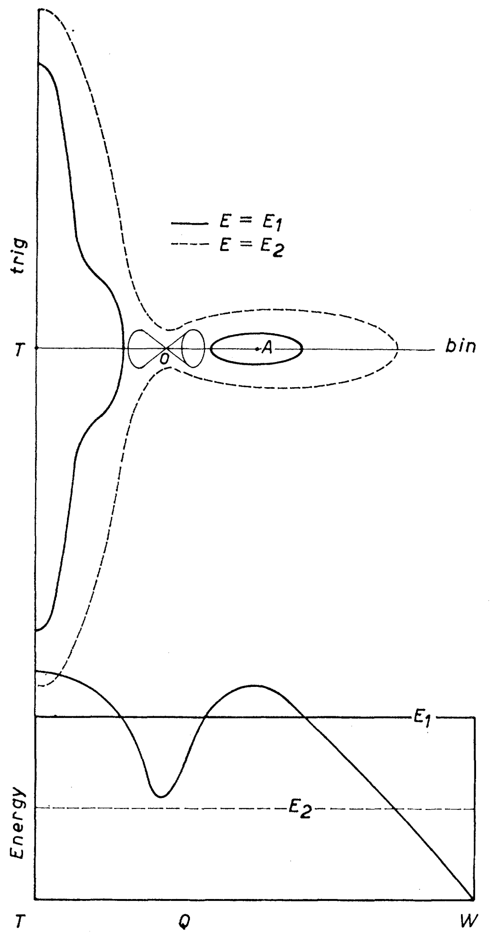

FIG. 8. Schematic representation of the holes band structure of bismuth (lower) and the energy-constant surface outline for two values of the energy in the trigonal binary plane (upper).

shown in Figs. 3 and 4 for this new pocket of carriers. With the notation

$$1=(\hbar^2/2m_0\epsilon_F)[\beta_1k_1^2+\beta_2k_2^2+\beta_3k_3^2], \tag{9}$$

where m_0 is the rest mass of the electron, a least-square fit gives for the coefficients the values

$$\frac{\hbar^2\beta_1}{2m_0\epsilon_F}=\frac{\hbar^2\beta_3}{2m_0\epsilon_F}=4\times10^{-12}\text{ cm}^2,\qquad \frac{\hbar^2\beta_2}{2m_0\epsilon_F}=3.2\times10^{-14}\text{ cm}^2. \tag{10}$$

In Fig. 7 the cross-section areas obtained by the Eq. (9) are reported for the normals to the intersecting planes lying in the binary-bisector and in the trigonal-binary planes. The dots give the experimental results. It is also to be noted that the ellipsoid is of rotation around the binary axis as the Baldareschi and Bassani[7] cone.

A schematic picture summarizing the interpretation of experimental results is given in Fig. 8, in which the band structure is presented in the lower part along the binary direction around the Fermi energy as given by Golin; in the upper part the energy-constant surface outline is shown for two values of the energy ϵ_1 and ϵ_2, where ϵ_1 is near to the Fermi energy.

5. CONCLUSIONS

The essential points of this work can be summarized as follows:

(1) the existence in the **k** space of a singular point of the saddle type;

(2) the variation of the phase factor γ from the value $\frac{3}{4}$ to the value $\frac{1}{2}$ is a consequence of the existence of this singular point;

(3) the appearance of a new type of holes when the Fermi level is lowered;

(4) the Landau-level splitting is the same as the spin splitting for this new pocket; and

(5) the experimental results are consistent with the band calculation carried out by Golin.

ACKNOWLEDGMENTS

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