QUASICLASSICAL QUANTIZATION OF ELECTRONS AND HOLES IN BISMUTH IN A MAGNETIC FIELD

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The asymptotic behavior of the eigenvalues of a system of four differential equations has been obtained in order to determine the splitting in a magnetic field of levels degenerate with respect to spin. The large magnitude of the splitting which (in order of magnitude) exceeds by a factor of m_0/m the splitting $2\mu H$ for a free electron is characteristic both for electrons and for holes. The values of the parameters for the bismuth spectrum determined previously [5] are used in the calculations of the dependence of the spin splitting on the direction of the magnetic field (Figs. 1 and 2).

1. It is well known [1] that the energy levels of electrons and of holes in a metal whose space lattice has a center of inversion are twofold degenerate. This degeneracy, which is analogous to the spin degeneracy for a free electron, is removed by the application of a magnetic field. As long as the magnetic field is weak the corresponding splitting is small and in order to calculate it one can utilize the quasiclassical approximation carrying out an expansion in powers of $\hbar$.

In the first approximation one obtains the quantization condition [2]

$$\frac{c}{e\hbar H}S(\varepsilon, k_{z'}) = 2\pi n,$$

which follows directly from the commutation relation

$$\{\hat{k}_{x'}, \hat{k}_{y'}\} = ie\hbar H/c, \quad \hat{\mathbf{k}} = -i\hbar\nabla - e\mathbf{A}/c.$$

Here $S(\epsilon, k_{z'})$ is the area of the intersection of the surface $\epsilon(\mathbf{k}) = \epsilon = \text{const}$ by the plane $k_{z'} = \text{const}$, the z' axis is chosen to lie along the magnetic field, n is an integer.

The result of the next approximation is fairly obvious:

$$\frac{c}{e\hbar H}S(\varepsilon, k_{z'}) \pm \frac{\pi}{2}g(\varepsilon, k_{z'}) = 2\pi\left(n + \frac{1}{2}\right).$$

It goes over into the well known expression which determines the free electron levels if we set $g(\epsilon, k_{z'}) = 2$ and take into account that $S(\epsilon, k_{z'}) = \pi(2m_0\epsilon - k_{z'}^2)$. The function $g(\epsilon, k_{z'})$ characterizing the "spin" splitting can be found in the case of metals of the type of bismuth the energy spectrum of which in the absence of a magnetic field was obtained in the paper by Abrikosov and the author [3].

Utilizing the results of the reference cited above [3], the author had earlier attempted [4] to calculate the energy spectrum in the presence of a magnetic field. In the resulting equations the magnetic field appears in two ways: first, through the operators $\hat{\mathbf{k}}$, and second, explicitly, describing in a certain sense the interaction with the magnetic moment of a free particle. We have succeeded in solving these equations exactly only for the case of holes and for a particular direction of the magnetic field. For an arbitrary direction we have discussed in the quasiclassical approximation only the explicit dependence on the field which, as has now become clear, leads to a relatively small splitting of the levels—of the order of magnitude of the splitting for a free electron μH (μ is the Bohr magneton). Below, neglecting this small splitting, we carry out a calculation of the function $g(\epsilon, k_{z'})$. It has turned out that $g(\epsilon, k_{z'})$ is of the order of magnitude unity, while the splitting is of the order of magnitude $m_0\mu H/m$, which appreciably exceeds μH due to the smallness of the effective masses m of the carriers in Bi.

2. One of the equations, or more accurately the system of four equations determining the spectrum of the electrons in a magnetic field, has the form

$$(\mathbf{V}\hat{\mathbf{k}} + \Gamma - \varepsilon)\Psi = 0. \qquad (1)$$

The functions Ψ are labelled by the subscript i ($i = 1, 2, 3, 4$) which we omit together with the matrix subscripts on V and Γ; a summation over one of them is implied in (1). The second equation is obtained from (1) by changing the sign of the constant Δ of the spin-orbit interaction on which the matrix Γ depends. The explicit form of the matrices is given in Sec. 3. One can easily convince

oneself that in the absence of a magnetic field both equations have the same eigenvalues.

We seek Ψ in the form

$$\Psi = \Phi e^{is/\hbar},$$

where the function s is assumed to be common to all the four functions Ψ. For Φ we obtain

$$[\mathbf{V}(\mathbf{k} - i\hbar\nabla) + \Gamma - \varepsilon]\Phi = 0, \tag{2}$$

$$\mathbf{k} = \nabla s - ec^{-1}\mathbf{A}. \tag{3}$$

We seek Φ in the form of a series in powers of $\hbar/i$

$$\Phi = \sum_{m=0}^{\infty} \left(\frac{\hbar}{i}\right)^m \varphi_m.$$

Comparing in (2) terms involving the same powers of $\hbar$ we obtain

$$(\mathbf{V}\mathbf{k} + \Gamma - \varepsilon)\varphi_m = -\mathbf{V}\nabla\varphi_{m-1}. \tag{4}$$

For m = 0 we obtain a homogeneous system of algebraic equations which has a solution under the condition

$$\mathrm{Det}(\mathbf{V}\mathbf{k} + \Gamma - \varepsilon) = 0. \tag{5}$$

The latter equation is the Hamilton-Jacobi equation in our approximation. The general solution of (4) for m = 0 has the form

$$\varphi_0 = C\varphi,$$

where φ is a solution.[1)]

We now discuss (4) for m = 1. The resultant equation has a solution under the condition

$$\bar{\varphi}\mathbf{V}\nabla C\varphi = 0, \qquad \bar{\varphi}(\mathbf{k}) = \varphi^*(\mathbf{k}^*). \tag{6}$$

Equation (6) determines the function C. For its solution it is useful to note (cf. the Appendix) that

$$\bar{\varphi}\mathbf{V}\varphi = \varphi\varphi\mathbf{v}.$$

Here $\mathbf{v} = \partial\epsilon/\partial\mathbf{k}$.

It is convenient to choose the vector potential in the form $A_{y'} = A_{z'} = 0$, $A_{x'} = -Hy'$. Then φ and C can be regarded as being independent of x' and z', and s can be sought in the form

$$s = x'K_{x'} + z'K_{z'} + \sigma(y')$$

with constant $K_{x'}$ and $K_{z'}$, as a result of which (3) goes over into

$$k_{x'} = K_{x'} + eHy'/c, \quad k_{y'} = d\sigma/d_{y'}, \quad k_{z'} = K_{z'}.$$

These equations enable us to use the variable $k_{x'}$ instead of y'.

Equation (5) for fixed ϵ and $k_{z'}$ determines the relationship $k_{y'}(k_{x'})$, i.e., the trajectory of the particle in momentum space. With its aid we obtain

$$\sigma = \frac{c}{eH}\int k_{y'}dk_{x'}.$$

The solution of (6) can be conveniently represented in the form

$$C = c_0(\bar{\varphi}\varphi v_{y'})^{-1/2}e^{-i\theta},$$

$$\theta = \frac{1}{2i}\int \frac{dk_{x'}}{\bar{\varphi}\varphi v_{y'}}\left(\bar{\varphi}V_{y'}\frac{d\varphi}{dk_{x'}} - \frac{d\bar{\varphi}}{dk_{x'}}V_{y'}\varphi\right). \tag{7}$$

In future we shall be interested in the "turning points" at which $v_{y'} = 0$. At the turning point a singularity arises in C, due to the presence of $v_{y'}$ in the factor preceding the exponential, and in order to go around this point we shall have to go over to complex values of k. All the other quantities in (7) are not singular at $v_{y'} = 0$, and, therefore, from the start it is sufficient to consider them only for real values of k. In this case the expression for θ can be transformed with the aid of the equation (cf. the Appendix)

$$\mathrm{Im}\,[d\varphi^*(v_{y'}V_{x'} - v_{x'}V_{y'})\varphi] = 0$$

to a form which does not depend on the choice of the vector potential

$$\theta = -\frac{1}{2}\,\mathrm{Im}\int \frac{dk}{v|\varphi|^2}\varphi^*\left(V_{x'}\frac{d}{dk_{y'}} - V_{y'}\frac{d}{dk_{x'}}\right)\varphi;$$

$$dk = [(dk_{x'})^2 + (dk_{y'})^2]^{1/2}, \quad v = (v_{x'}^2 + v_{y'}^2)^{1/2}.$$

Since in bismuth closed equal-energy surfaces are of interest, the corresponding trajectories are closed curves. This means that there exist several (at least two) branches $k_{y'}^{(\alpha)}(k_{x'})$ ($\alpha = 1, 2, \ldots$). At the turning points the two branches merge becoming complex in the classically inaccessible region of values of $k_{x'}$. In the classically accessible region the function Ψ is a linear combination of the functions Ψ defined on the branches $k_{y'}^{(\alpha)}$. For $k_{x'} \to \pm\infty$ the choice of the branch is determined by the condition that Ψ should be finite.

It is now easy to formulate the condition of quantization. We choose a certain point $(k_{x'}, k_{y'})$ on the trajectory and observe the variation of Ψ in moving along this trajectory. After a complete circuit the quantity s will acquire an increment $(c/eH)s(\epsilon, k_{z'})$; we denote the increment in the quantity θ by $\frac{1}{2}\pi g(\epsilon, k_{z'})$. It remains now to find the value of the increment arising from the factor preceding the exponential in C (7). In order to do this we shall go around the turning points, penetrating into the classically inaccessible region, in

[1)] We do not consider the possible existence of two independent solutions, which can be realized only at isolated points.

order to make a unique choice of the branch. It is essential for the argument that in the neighborhood of a "turning point" $v_{y'}$ can be represented by the expansion $v_{y'} = l(k_{y'} - k_{y'}^{(0)})$. Thus, in going over, for example, from positive to negative values of $k_{y'} - k_{y'}^{(0)}$ the quantity $\ln\sqrt{v_{y'}}$ acquires an increment $\pm\pi/2$ depending on whether we are dealing with the right-hand or the left-hand turning point. Further, since $\epsilon(\mathbf{k}) = \epsilon(-\mathbf{k})$, there exists an even number of turning points, while at points obtained from one another by inversion the increment of $\ln\sqrt{v_{y'}}$ has the same sign.

Since Ψ must be unique, we obtain up to terms in $\hbar^2$ the relation given in Sec. 1 with the function $g(\epsilon, k_{z'})$ being determined by the equation

$$g(\varepsilon, k_{z'}) = \frac{1}{\pi}\operatorname{Im}\oint \frac{dk}{v|\varphi|^2}\varphi^*\left[\mathbf{V}\frac{d}{d\mathbf{k}}\right]_{z'}\varphi. \qquad (8)$$

The fact that the function $g(\epsilon, k_{z'})$ appears in the condition of quantization with the sign $\pm$ is explained by the existence of two equations which go over into one another under the replacement $\Delta \to -\Delta$.

The condition for the validity of the quasiclassical approximation is $ehH/2\pi cS \ll 1$. With the same degree of accuracy we obtain by a direct differentiation the change in energy $\Delta\epsilon$ in transitions in which the quantum numbers $k_{z'}$ and n are unchanged (with only the "spin" quantum number undergoing a change)

$$\Delta\varepsilon = e\hbar Hg(\varepsilon, k_{z'})\,/\,2m(\varepsilon, k_{z'})c,$$
$$m(\varepsilon, k_{z'}) = \frac{1}{2\pi}\frac{\partial S(\varepsilon, k_{z'})}{\partial\varepsilon}. \qquad (9)$$

It is natural to call the quantity $2m(\epsilon, k_{z'})/|g(\epsilon, k_{z'})|$ the "spin" mass. Formula (9) explains the experimentally observed equality (in order of magnitude) of the "spin" and the "orbital" masses—anomalously small orbital masses correspond to small spin masses. This situation is possible because, as we shall see below, $g(\epsilon, k_{z'})$ is of order of magnitude unity.

3. For the evaluation of the function $g(\epsilon, k_{z'})$ for electrons we utilize the following representation of the matrices $\mathbf{V}$ and Γ [4]:

$$V_x = b\begin{vmatrix}\sigma_y & 0\\ 0 & -\sigma_y\end{vmatrix},\quad V_y = b\begin{vmatrix}\sigma_z & 0\\ 0 & \sigma_z\end{vmatrix},\quad V_z = a\begin{vmatrix}1 & 0\\ 0 & -1\end{vmatrix},$$

$$\Gamma = \begin{vmatrix}\beta^{(1)} & \Delta & 0 & \gamma_+\\ \Delta & -\beta^{(1)} & -\gamma_- & 0\\ 0 & -\gamma_- & -\beta^{(1)} & -\Delta\\ \gamma_+ & 0 & -\Delta & \beta^{(1)}\end{vmatrix}.$$

Here σ_y and σ_z are the Pauli matrices, 0 in V_x, V_y, V_z and 1 in V_z are two-rowed matrices:

$$0 = \begin{vmatrix}0 & 0\\ 0 & 0\end{vmatrix},\quad 1 = \begin{vmatrix}1 & 0\\ 0 & 1\end{vmatrix};$$

a, b, Δ, $\beta^{(1)}$, γ_+, and γ_- are constants. The coordinate axes are chosen as follows: the x axis along the binary axis C_2, and the z axis makes an angle $\arccos\frac{1}{3}$ with the trigonal axis C_3 of the crystal. We consider one of the three groups of electrons. The C_2 axis for this group is a twofold symmetry axis [5].

We choose for φ the co-factors of the elements of the first row of the matrix $|\mathbf{k}\cdot\mathbf{V} + \Gamma - \epsilon|$:

$$\varphi^{(1)} = (k_3 + \Omega_+)[\Delta^2 + k_1^2 + (k_2 + \Omega_-)(k_3 - \Omega_+)] + \gamma_-^2(k_2 + \Omega_-),$$
$$\varphi^{(2)} = (\Delta + ik_1)[\Delta^2 + k_1^2 + (k_2 + \Omega_-)(k_3 - \Omega_+)] + \gamma_+\gamma_-(-\Delta + ik_1),\quad \varphi^{(3)} = \gamma_+(\Delta - ik_1)(k_3 + \Omega_+) + \gamma_-(\Delta + ik_1)(k_2 + \Omega_-),\quad \varphi^{(4)} = \gamma_+(\gamma_-^2 + k_3^2 - \Omega_+^2) - \gamma_-(\Delta + ik_1)^2;\quad \Omega_\pm = \varepsilon \pm \beta^{(1)},\quad k_1 = bk_x,$$
$$k_{2,3} = bk_y \pm ak_z.$$

The following value of $|\varphi|^2$ corresponds to the above choice:

$$|\varphi|^2 = \sum_{i=1}^{4}|\varphi^{(i)}|^2$$
$$= 2[(\Omega_- + k_2)(\gamma_-^2 + k_3^2 - \Omega_+^2) + (\Omega_+ + k_3)(\Delta^2 + k_1^2)]$$
$$\times[(\Omega_+ + \Omega_-)(\Delta^2 + k_1^2) + \Omega_-(k_3^2 + \gamma_-^2 - \Omega_+^2) + \Omega_+(k_2^2 + \gamma_+^2 - \Omega_-^2)].$$

Equation (5) relating k_1, k_2, and k_3, can be solved for k_1:

$$k_1^2 = \Omega_+\Omega_- - \gamma_+\gamma_- - \Delta^2 - k_2k_3 + \sqrt{u}, \qquad (10)$$

where we have used the notation

$$u = (\Omega_-\gamma_- - \Omega_+\gamma_+)^2 + 4\Delta^2\gamma_+\gamma_- - (\gamma_-^2 - \Omega_+^2)k_2^2 - (\gamma_+^2 - \Omega_-^2)k_3^2 + 2(\gamma_-\gamma_+ - \Omega_-\Omega_+)k_2k_3.$$

We introduce the unit vector $\mathbf{n}$ directed along the magnetic field. From (10) and

$$\mathbf{kn} = k_{z'} = \text{const} \qquad (11)$$

we obtain the differential equation for the trajectory

$$\frac{dk_1}{v_2n_3 - v_3n_2} = \frac{dk_2}{v_3n_1 - v_1n_3} = \frac{dk_3}{v_1n_2 - v_2n_1},$$

where n_α ($\alpha = 1, 2, 3$) are related to the Cartesian

components of the vector n

$$n_1 = 2an_x, \quad n_{2,3} = an_y \pm bn_z.$$

a) Let us consider the case $n_X = 0$. The magnetic field lies in the plane perpendicular to the C_2 axis. We use as our starting point

$$g(\varepsilon, k_{z'}) = \frac{2}{\pi} \operatorname{Im} \oint dk_2 \frac{\varphi^* V_x d\varphi/dk_2}{|\varphi|^2 v_x}$$
$$= \frac{2}{\pi} \operatorname{Im} \oint \frac{dk_2}{n_3 b v_1 |\varphi|^2} \varphi^* V_x \left(n_3 \frac{\partial}{\partial k_2} - n_2 \frac{\partial}{\partial k_3} \right) \varphi.$$

Evaluating

$$\operatorname{Im} \varphi^* V_x \frac{\partial \varphi}{\partial k_2} = 2\Delta b \gamma_- [\gamma_- (-\gamma_-\gamma_+ + \Omega_-\Omega_+ - k_2k_3)$$
$$- \gamma_+ (\gamma_-^2 + k_3^2 - \Omega_+^2) + \gamma_- \sqrt{u}],$$
$$\operatorname{Im} \varphi^* V_x \frac{\partial \varphi}{\partial k_3} = 2\Delta b [k_3^2 \Omega_-^2 - k_2^2 (\gamma_-^2 - \Omega_+^2)$$
$$+ k_2k_3 (3\gamma_-\gamma_+ - 2\Omega_-\Omega_+) + (\gamma_+\Omega_+ - \gamma_-\Omega_-)(\gamma_+k_3 + \gamma_-k_2)$$
$$+ \gamma_+^2\Omega_+^2 + 2\gamma_-^2\gamma_+^2 - 3\gamma_-\gamma_+\Omega_-\Omega_+ + 4\Delta^2\gamma_-\gamma_+$$
$$+ (\Omega_-k_3 - \Omega_+k_2 - 3\gamma_-\gamma_+)\sqrt{u}]$$

and eliminating k_3 by means of

$$k_3 = n_3^{-1}(-n_2k_2 + 2abk_{z'}), \tag{12}$$

we obtain for $g(\epsilon, k_{z'})$ an expression which reduces to elliptic integrals. It has a fairly simple form for $k_{z'} = 0$:

$$g(\varepsilon, 0) = \frac{2\Delta}{\pi D} \int_{-t_1}^{t_1} dt \frac{L + Mt + Nt^2}{w(-1 + n_2n_3t^2 + w)^{1/2}(P + Qt + Rt^2)},$$
$$w = \left[\frac{(\gamma_-\Omega_- - \gamma_+\Omega_+)^2 + 4\Delta^2\gamma_-\gamma_+}{D^2} - t^2 \right.$$
$$\left. \times \frac{n_3^2(\gamma_-^2 - \Omega_+^2) + n_2^2(\gamma_+^2 - \Omega_-^2) + 2n_2n_3(\gamma_-\gamma_+ - \Omega_-\Omega_+)}{D} \right]^{1/2} \tag{13}$$

$$L = n_2(-3Dw\gamma_-\gamma_+ + \Omega_+^2\gamma_+^2 + 2\gamma_-^2\gamma_+^2 - 3\Omega_-\Omega_+\gamma_-\gamma_+$$
$$+ 4\Delta^2\gamma_-\gamma_+) - n_3(Dw\gamma_-^2$$
$$+ \gamma_-^2\Omega_-\Omega_+ - 2\gamma_-^3\gamma_+ + \gamma_-\gamma_+\Omega_+^2),$$
$$M = n_2\sqrt{D}[Dw(\Omega_-n_2 + \Omega_+n_3) + (\gamma_+\Omega_+ - \gamma_-\Omega_-)$$
$$\times (\gamma_+n_2 - \gamma_-n_3)], \quad N = n_2D[n_2^2\Omega_-^2 - n_3^2(2\gamma_-^2 - \Omega_+^2)$$
$$- 2(\gamma_-\gamma_+ - \Omega_-\Omega_+)n_2n_3], \quad P = Dw\Omega_+ + \Omega_-\gamma_-^2$$
$$- \Omega_+\gamma_-\gamma_+,$$
$$Q = \sqrt{D}[(Dw + \Omega_-\Omega_+ - \gamma_-\gamma_+)n_2 - (\gamma_-^2 - \Omega_+^2)n_3],$$
$$R = n_2D(\Omega_-n_2 - \Omega_+n_3), \quad D = \gamma_-\gamma_+ - \Omega_-\Omega_+ + \Delta^2;$$

$-1 + n_2n_3t_1^2 + w(t_1^2) = 0$ and a change of variables has been utilized

$$k_2 = -n_3\sqrt{D}t, \qquad k_3 = n_2\sqrt{D}t,$$

which takes (12) into account.

The quantity $g(\epsilon_f, 0)$ is of particular interest since the intersection of the Fermi surface by the plane $k_{Z'} = 0$ determines the nature of the oscillations of the magnetic susceptibility, conductivity, etc. A plot of $g(\epsilon_f, 0)$ against the direction of the magnetic field for $n_X = 0$ is shown in Fig. 1. For the calculation we have utilized the parameters of the bismuth spectrum obtained earlier[5]. We have restricted ourselves to the angular interval from 0 to π, since $g(\epsilon, k_{Z'})$ changes sign when the magnetic field changes sign. The reason for the sharp variations in g is that on the Fermi surface in the plane $k_X = 0$ there exist the two points which were mentioned in the first footnote.

b) We now consider the case $n_Y = n_Z = 0$. The magnetic field is directed along the second order axis. Representing $g(\epsilon, k_{Z'})$ in the form

$$g(\varepsilon, k_{z'}) = \frac{2}{\pi} \operatorname{Im} \oint dk_3 \frac{\varphi^* V_z d\varphi/dk_3}{|\varphi|^2 v_z}$$

and taking into account the fact that

$$v_z = \frac{\partial \varepsilon}{\partial k_z} = a\frac{\partial \varepsilon}{\partial k_2} - a\frac{\partial \varepsilon}{\partial k_3} = a(v_2 - v_3),$$
$$\frac{d}{dk_3} = \frac{\partial}{\partial k_3} - \frac{v_3}{v_2}\frac{\partial}{\partial k_2},$$

we obtain

$$g(\varepsilon, k_{z'}) = \frac{2}{\pi} \operatorname{Im} \oint \frac{dk_3}{a|\varphi|^2 v_2(v_2 - v_3)} \varphi^* V_z \left(v_2 \frac{\partial}{\partial k_3} - v_3 \frac{\partial}{\partial k_2} \right) \varphi.$$

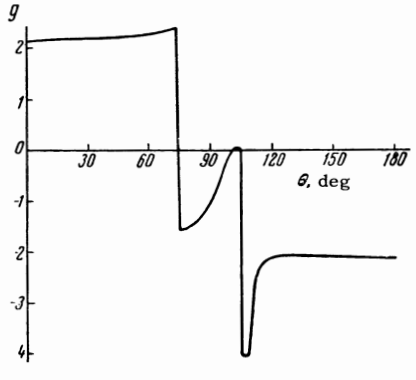

FIG. 1. The g-factor in the central section of the Fermi surface for electrons vs. the direction of the magnetic field. The magnetic field is in the plane perpendicular to the C_2 axis. The angle is measured from the "former" threefold axis. The directions of the C_1 and C_3 axes correspond to angles of 19.5° and 109.5°. The Fermi surface is elongated in the direction of the 13° angle.

Evaluating the derivatives

$$\operatorname{Im}\varphi^* V_z \frac{\partial\varphi}{\partial k_2} = -4\Delta\gamma_+\gamma_- k_1 k_3 a,$$

$$\operatorname{Im}\varphi^* V_z \frac{\partial\varphi}{\partial k_3} = -4\Delta\gamma_+\gamma_- k_1 k_3 a,$$

we obtain

$$g(\varepsilon, k_{z'}) = -\frac{8}{\pi}\Delta\gamma_+\gamma_- k_1 \oint \frac{k_3 dk_3}{v_2|\varphi|^2}. \qquad (14)$$

If now use (10) to express k_2 in terms of k_1 = const and k_3 and substitute in (14), then the corresponding integral will vanish due to the fact that the integrand is odd in k_3, so that in the case under consideration $g(\epsilon, k_{Z'}) = 0$.

c) The case of an arbitrary direction of the magnetic field. We write for $g(\epsilon, k_{Z'})$ the expression

$$g(\varepsilon, k_{z'}) = \frac{2}{\pi}\operatorname{Im}\oint dk_2 \frac{\varphi^* V_x d\varphi/dk_2}{|\varphi|^2 v_x},$$

which by means of straightforward transformations can be brought to the form

$$g(\varepsilon, k_{z'}) = \frac{2}{\pi}\operatorname{Im}\oint \frac{dk_2}{b(v_3 n_1 - v_1 n_3)|\varphi|^2} \times \varphi^*\left(n_2 V_x \frac{\partial}{\partial k_3} - n_3 V_x \frac{\partial}{\partial k_2} + n_1 V_y \frac{\partial}{\partial k_2}\right)\varphi. \qquad (15)$$

The averages appearing in the above expression are equal to

$$\operatorname{Im}\varphi^* V_x \frac{\partial\varphi}{\partial k_3} = b\Delta\{[\Delta^2 + k_1^2 + (k_2 + \Omega_-)(k_3 - \Omega_+)]^2 - 4k_1^2\gamma_+\gamma_- - \gamma_+^2\gamma_-^2 - \gamma_-^2(k_2 + \Omega_-)^2 + \gamma_+^2(k_3 + \Omega_+)^2\},$$

$$\operatorname{Im}\varphi^* V_x \frac{\partial\varphi}{\partial k} = 2b\Delta\gamma_-\{\gamma_-(\Delta^2 + k_1^2) - \gamma_+(\gamma_-^2 - \Omega_+^2 + k_3^2)\}, \quad \operatorname{Im}\varphi^* V_y \frac{\partial\varphi}{\partial k_2} = 4b\Delta\gamma_+\gamma_- k_1 k_3.$$

It is not possible to simplify (15) further since we have not succeeded in the general case in expressing k_1 and k_3 in terms of k_2 from (10) and (11).

4. The function $g(\epsilon, k_{Z'})$ for holes can be obtained from (15) by means of the substitution

$$\gamma_+ \to \gamma, \quad \gamma_- \to \gamma, \quad \beta^{(1)} \to 0$$

and a transition to a coordinate system in which the z axis coincides with the trigonal axis of the crystal (Fig. 2). However, as has been shown earlier[5], the hole spectrum in the absence of a magnetic field is very close to quadratic. This fact enables us to use a different method of solving Eqs. (1), now written in the form[4]

$$\begin{pmatrix} a\hat{k}_z + \Delta - \Omega & b\hat{k}_+ & \gamma & 0 \\ b\hat{k}_- & a\hat{k}_z - \Delta - \Omega & 0 & \gamma \\ \gamma & 0 & -a\hat{k}_z + \Delta - \Omega & -b\hat{k}_+ \\ 0 & \gamma & -b\hat{k}_- & -a\hat{k}_z - \Delta - \Omega \end{pmatrix} \begin{vmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \varphi_4 \end{vmatrix} = 0,$$

$$\hat{k}_\pm = \hat{k}_y \pm i\hat{k}_x. \qquad (16)$$

We obtain φ_3 and φ_4 from the first and the second equations of system (16) and substitute them into the third and the fourth equations:

$$[\gamma^2 - (\Delta - \Omega)^2 + a^2\hat{k}_z^2 + b^2\hat{k}_+\hat{k}_-]\varphi_1 + (-2b\Delta\hat{k}_+ + ab\hat{k}_z\hat{k}_+ + ab\hat{k}_+\hat{k}_z)\varphi_2 = 0,$$

$$(2b\Delta\hat{k}_- + ab\hat{k}_-\hat{k}_z + ab\hat{k}_z\hat{k}_-)\varphi_1 + [\gamma^2 - (\Delta + \Omega)^2 + a^2\hat{k}_z^2 + b^2\hat{k}_-\hat{k}_+]\varphi_2 = 0. \qquad (17)$$

Since the Fermi level lies very near to the top of the band which is determined by the equation $\bar{\Omega} = \Delta - |\gamma|$, while k^2 is of order of magnitude $\gamma^2 - (\Delta - \Omega)^2$ (for the sake of definiteness we take Δ to be positive), we can neglect the terms $a^2\hat{k}_z^2 + b^2\hat{k}_-\hat{k}_+$ and $ab\hat{k}_-\hat{k}_z + ab\hat{k}_z\hat{k}_-$ in the second equation and $ab\hat{k}_z\hat{k}_+ + ab\hat{k}_+\hat{k}_z$ in the first equation. After this problem reduces to the solution of the one equation:

$$[2|\gamma|(\Omega - \Delta + |\gamma|) + a^2\hat{k}_z^2 + \frac{|\gamma|}{|\gamma| - \Delta} b^2 k_+ k_-]\varphi_1 = 0. \qquad (18)$$

Equation (18) can be conveniently solved using the vector potential $A_{X'} = A_{Z'} = 0$, $A_{Y'} = Hx'$. Noting that

$$\hat{k}_\pm = \hat{k}_{y'}\cos\theta + \hat{k}_{z'}\sin\theta \pm i\hat{k}_x = (k_{y'} - eHx'/c)\cos\theta + k_{z'}\sin\theta \pm \hbar\partial/\partial x',$$

$$\hat{k}_z = -(k_{y'} - eHx'/c)\sin\theta + k_{z'}\cos\theta$$

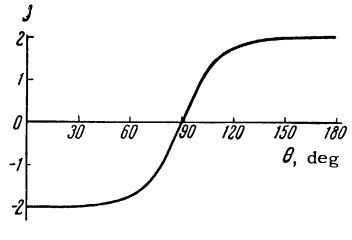

FIG. 2. The g-factor for holes vs. the direction of the magnetic field. The angle is measured from the trigonal axis.

($k_{y'}$, $k_{z'}$ are constants, θ is the angle between the magnetic field and the C_3 axis) we obtain

$$k_+k_- = -\hbar^2\frac{\partial^2}{\partial x^2}+\left[\left(k_{y'}-\frac{eHx'}{c}\right)\cos\theta+k_{z'}\sin\theta\right]^2 - \frac{eH\hbar}{c}\cos\theta.$$

Carrying out an analogous calculation for the system obtained from (17) by the replacement $\Delta \to -\Delta$, we obtain an equation which differs from (18) by the interchange of k_+ and k_-. Noting that the expression for $\hat{k}_-\hat{k}_+$ differs from $\hat{k}_+\hat{k}_-$ only by the sign of the last term we obtain the spectrum

$$\Omega-\bar{\Omega}=\frac{e\hbar H}{c}\left[\left(n+\frac{1}{2}\right)\frac{1}{m(\theta)}\pm\frac{\cos\theta}{2m(0)}\right] + \frac{k_{z'}^2m^2(\theta)}{2m(0)m^2(\pi/2)}, \qquad (19)$$

where $m(\theta)$ is the cyclotron mass

$$m(\theta)=\frac{\bar{\Omega}}{b^2}\left(\cos^2\theta-\frac{a^2\bar{\Omega}}{b^2|\gamma|}\sin^2\theta\right)^{-1/2}.$$

From (19) it follows that in the case when the magnetic field is perpendicular to the C_3 axis the "spin" splitting is equal to zero, while in a field directed along the trigonal axis it is equal to the orbital splitting.

We note that Smith et al.[6] did in fact observe a small splitting in the first case. However, in the second case they had to assume that the magnitude of the spin splitting exceeds the orbital splitting by a factor two.

There is a way of making the dependence of the g-factor on the direction of the magnetic field continuous (Fig. 1). In order to do this we must ascribe the discontinuity in g to the quantum number n (cf., Sec. 1), by replacing n by $n \pm 1$ on one side of the discontinuity. Then the left hand side of Fig. 1 ($0 < \theta < 75°$) will be lowered and the right hand side ($105° < \theta < 180°$) will be raised by four. A continuous variation both of the g factor and of the number n corresponds to a different way of going around the zeros of $|\varphi|^2$ in the complex k_2 plane (Sec. 3a).

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APPENDIX

1. We now give a proof of the relation $\bar{\varphi}\mathbf{V}\varphi = \bar{\varphi}\varphi\mathbf{v}$. Differentiating (4) for $m = 0$ with respect to k and multiplying on the left by $\bar{\varphi}$, we obtain

$$\bar{\varphi}\left(\mathbf{V}-\frac{\partial\varepsilon}{\partial\mathbf{k}}\right)\varphi+\varphi(\mathbf{V}\mathbf{k}+\Gamma-\varepsilon)\frac{\partial\varphi}{\partial\mathbf{k}}=0.$$

Utilizing the hermiticity of V and Γ we obtain the desired result.

2. We now give a proof that $\mathrm{Im}[\varphi^*(v_{y'}V_{x'}-v_{x'}V_{y'})d\varphi] = 0$. We differentiate (4) for $m = 0$ with respect to $\mathbf{k}$ along the trajectory, i.e., for $\epsilon = \text{const}$, $k_{z'} = \text{const}$ and we multiply on the left by $d\varphi^*$

$$d\varphi^*(V_{x'}dk_{x'}+V_{y'}dk_{y'})\varphi+d\varphi^*(\mathbf{V}\mathbf{k}+\Gamma-\varepsilon)d\varphi=0,$$

from which the required relation follows since

$$\mathrm{Im}[d\varphi^*(\mathbf{V}\mathbf{k}+\Gamma-\varepsilon)d\varphi]=0,$$

$$d\varepsilon=v_{x'}dk_{x'}+v_{y'}dk_{y'}=0.$$

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