The electron *g* factor for one-band and two-band extended models of electron energy spectrum

G.P. Mikitik and Yu.V. Sharlai

B. Verkin Institute for Low Temperature Physics and Engineering
of the National Akademy of Sciences of Ukraine, 47 Lenin Ave., Kharkov 61103, Ukraine
E-mail: sharlai@ilt.kharkov.ua

At present, *explicit* expressions for the electron *g* factor in crystals are known only for the following two cases: either the Fermi energy ε_F of the electrons lies at the edge of the electron energy band, $\varepsilon(\mathbf{k}_{ex})$, or the electron energy spectrum of a crystal can be approximated by the two-band model. Here we obtain explicit formulas for the *g* factor in situations when the Fermi level ε_F is close to but does not coincide with the band edge and when the two-band model of the spectrum includes small corrections from other electron energy bands. In particular, we derive the expression that describe the dependences of the *g* factor on $\varepsilon_F - \varepsilon(\mathbf{k}_{ex})$ and on the direction of the magnetic field for doped semiconductors. The results are applied to III−V semiconductors and to bismuth.

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1. Introduction

As is well known [1], the *g* factor of electrons in crystals with inversion symmetry specifies the splitting of Landau energy levels caused by an interaction of the electron spin with a magnetic field, $\Delta E = g(e\hbar/2mc)H$, and can considerably differ from its free-electron value, $g = 2$. Here e and m are the charge and mass of an electron, and H is the external magnetic field. In this paper we shall discuss the *g* factors in the semiclassical limit when there are many Landau levels under the Fermi surface of the crystal. Besides this, we exclude from consideration those situations in which magnetic breakdown occurs. In this case the semiclassical *g* factor appears in the well-known quantization rule [1−4] for electron energy ε in a magnetic field,

$$S(\varepsilon, k_H) = 2\pi \frac{|e|H}{\hbar c}\left(n + \gamma \pm \frac{g(\varepsilon, k_H)m^*}{4m}\right), \quad (1)$$

where S is the cross-sectional area of the closed semiclassical orbit Γ of the electron in the Brillouin zone, k_H is the component of the wave vector of the electron in the direction of the external magnetic field $\mathbf{H}$, n is a large integer, the cyclotron mass $m^* = (\hbar^2/2\pi)(\partial S(\varepsilon, k_H)/\partial\varepsilon)$, the constant γ is always

equal to $1/2$ when the spin−orbit interaction is taken into account [5,6], and the *g* factor $g(\varepsilon, k_H)$ depends on the location of the orbit Γ in the Brillouin zone [7].

The exact equations for the *g* factor were derived in Refs. [5,8]. (In fact, they are another representation of Roth prime s results [9].) These equations take into account the dynamics of the electron spin when the electron moves in its semiclassical orbit. For this reason the *g* factor depends on the entire orbit and is usually not expressed in explicit form. On the other hand, in many papers, see, e.g., Refs. [10−26], the so-called local *g* factors $g(\mathbf{k})$ introduced by De Graaf and Overhauser [27] for points $\mathbf{k}$ on the Fermi surface were calculated, and the *g* factor of the orbit was obtained by integration of $g(\mathbf{k})$ over the orbit. In this symplified approach the dynamics of the electron spin is neglected completely. As was shown in our previous papers [8,28], the symplified approach is approximately valid if the spin−orbit interaction in the crystal is not too strong. Besides this, at an arbitrary strength of this interaction there are two situations when the symplified approach leads to the exact result for the *g* factor.

In the first situation, which is characteristic, e.g., for doped semiconductors, the Fermi level of the electrons practically coincides with a minimum (or a max-

imum) of the electron energy band $\varepsilon(\mathbf{k})$, and hence this $\varepsilon(\mathbf{k})$ can be well approximated by the «one-band» model,

$$\varepsilon(\mathbf{k}) \approx \varepsilon(\mathbf{k}_{ex}) + \sum_{\alpha = x,y,z} \frac{\hbar^2 (k_\alpha - k_{ex,\alpha})^2}{2m_\alpha}, \quad (2)$$

where $\mathbf{k}_{ex}$ is the point of the energy-band extremum in the Brillouin zone, and m_α are all positive (or negative) effective masses at this point. In this case the electron orbit takes the shape of a very small ellipse surrounding the point $\mathbf{k}_{ex}$, and the g factor of the orbit coincides to a first approximation with the local g factor $g(\mathbf{k}_{ex})$.

In the second situation the electron energy spectrum of the crystal can be well approximated by the two-band model [28]. The two-band model can be applied to the description of the energy spectrum if in some region of the Brillouin zone the energy gap between the band under consideration and some other band as well as the energy differences between these bands and the Fermi energy ε_F are all relatively small as compared to other energy gaps in the crystal. (Then one may consider only these two bands, neglecting the other bands of the crystal.) In this case the energy dispersion relations $\varepsilon(\mathbf{k})$ for both the bands are found from a quadratic equation that can be always reduced to the form:

$$\left[\varepsilon - \frac{[\mathbf{v}_0(0) + \mathbf{v}_a(0)]\mathbf{k}}{2} \right]^2 =$$

$$= \left[\frac{E_g}{2} + \frac{[\mathbf{v}_0(0) - \mathbf{v}_a(0)]\mathbf{k}}{2} \right]^2 + q_1^2 k_x^2 + q_2^2 k_y^2 + q_3^2 k_z^2, \tag{3}$$

where $\mathbf{v}_0(0)$, $\mathbf{v}_a(0)$, q_1, q_2, q_3 are some real constants, and E_g is the energy gap between these bands at some point of the above-mentioned region of the Brillouin zone (this point is taken as $\mathbf{k} = 0$). For example, the electron energy spectrum of bismuth and its alloys near the point L of the Brillouin zone is close to this type. The two-band model can be also useful for narrow-gap semiconductors. In this two-band case the appropriate equation [8] determining the g factor can be solved explicitly [28], and the result for the g factor of the electron orbit (this orbit need not be small now) coincides with that obtained in the framework of the local g factor approach. Interestingly, in this case the combination $\delta \equiv gm^*/4m$ is equal to [29] $\pm 1/2$, i.e., the splitting of the electron energy levels in the magnetic field described by the g factor coincides exactly with their orbital splitting. This result generalizes the well-known finding of Cohen and Blount [30] obtained for a symplified variant of the two-band model [31].

The above exactly solvable cases can be applied to real situations only approximately. In particular, the Fermi energy in doped semiconductors does not lie strictly at the edge of the energy band, and thus the electron orbits have a small but finite size. In that case, the g factors of such orbits slightly differ from the g factor calculated at the edge of the band, $g(\mathbf{k}_{ex})$. Since g factors are measured with high accuracy [32,33], the correction $\Delta g \equiv g - g(\mathbf{k}_{ex})$ was experimentally investigated in a number of semiconductors [34]. It is clear that to calculate this correction, one has to go beyond the framework of the local g factor approach. As to the two-band model, it sufficiently well describes the energy spectrum of bismuth when the wave vector $\mathbf{k}$ is perpendicular to the longest axis of its Fermi surface at the point L, i.e., this model is good enough for magnetic fields directed along this axis. When the magnetic field deviates from the longest axis, corrections to the g of the two-band model have been observed experimentally in bismuth [35], and the accurate calculation of the g factor is possible only if one goes beyond the framework of the two-band model (and of the local g factor approach).

In this paper we consider one-band and two-band extended models of the electron spectrum which include small corrections to the above exactly solvable cases. These models enable one to describe the electron energy spectra in a number of real situations. In the framework of these extended models we find *explicit* formulas for the g factor, using the theory [8]. In particular, the case of doped semiconductors is analyzed in detail. As an illustration, the results obtained are applied to III−V semiconductors and to bismuth.

2. Calculation of the *g* factor

The g factor in the quantization rule (1) is expressed in terms of the matrix elements of the effective one-band Hamiltonian $\hat{H}_{eff}$ of a Bloch electron in a magnetic field. Since the electron bands are twofold degenerate in crystals with inversion symmetry [4], the Hamiltonian is a 2×2 matrix in the spinor space. This Hamiltonian to first order in the magnetic field H has the form [36,37]

$$\hat{H}_{eff} = \varepsilon(\hat{\mathbf{k}})\hat{\mathbb{1}} + \frac{e}{c} H \hat{\mu}(\hat{\mathbf{k}}, \mathbf{n}), \tag{4}$$

where $\mathbf{n}$ is the unit vector directed along the magnetic field $\mathbf{H}$, $\varepsilon(\mathbf{k})$ is the electron dispersion relation for the band being investigated, $\hat{\mathbf{k}} = \mathbf{K} - (e/c\hbar)\mathbf{A}(i\partial/\partial\mathbf{K})$, $\mathbf{A}(\mathbf{r})$ is the vector potential of the magnetic field $\mathbf{H}$, and the function $\varepsilon(\hat{\mathbf{k}})$ in Eq. (4) is assumed to be completely symmetrized in the components of $\hat{\mathbf{k}}$. The 2×2 matrix $[eH\hat{\mu}(\mathbf{k}, \mathbf{n})/c]$ describes the interaction of

the electron spin with the magnetic field in the crystal, and its elements satisfy the relation: $\mu_{11} = -\mu_{22}$, $\mu_{12} = \mu_{21}^*$. In Ref. 8 (Appendix) it was shown how to calculate this matrix explicitly when one starts from the so-called $\mathbf{k \cdot p}$ Hamiltonian [4] or from the Hamiltonian in the LMTO representation [38]. Dependences of the matrix $\hat{\mu}$ on $\mathbf{k}$ and on $\mathbf{n}$, up to numerical factors, can be also found using the theory of invariants [39].

In Appendix A of this paper we present the equations of Ref. 8 for the g factor and find the g factors for the one-band and two-band models of the spectrum. Let us denote the energy dispersion relation and the matrix μ for the energy band under consideration in these exactly solvable cases as $\varepsilon^{(0)}(\mathbf{k})$ and $\mu_{\rho\rho'}^{(0)}(\mathbf{k})$ ($\rho, \rho' = 1,2$). Below we shall consider the models for which one may write,

$$\varepsilon(\mathbf{k}) = \varepsilon^{(0)}(\mathbf{k}) + \Delta\varepsilon(\mathbf{k}), \qquad (5)$$

$$\mu_{\rho\rho'}(\mathbf{k}) = \mu_{\rho\rho'}^{(0)}(\mathbf{k}) + \Delta\mu_{\rho\rho'}(\mathbf{k}), \qquad (6)$$

where the terms $\Delta\varepsilon(\mathbf{k})$, $\Delta\mu_{\rho\rho'}(\mathbf{k})$ are small corrections. Assuming that these corrections are known, we shall find the appropriate corrections to the g factors of the electron orbits for these extended models. Note that the orbits are slightly deformed by the term $\Delta\varepsilon(\mathbf{k})$ in Eq. (5). The appropriate deformation is found in Appendix B.

To find the g factor, we have to solve Eq. (A.2). Note that it is always possible to reduce the matrix $c_{\rho\rho'}$ in Eq. (A.5) to diagonal form by a constant unitary transformation in the spinor space. Thus, without loss of generality we may assume that $c_{11} = -c_{22} = \lambda$, $c_{12} = c_{21} = 0$, with λ from Eq. (A.6). Then Eq. (A.2) takes the following form

$$i\frac{\hbar c}{|e|H}\tau = 2\lambda\tau\psi(\mathbf{k}) +$$

$$+ \Delta\mu_{12}(\mathbf{k})\tau^2 + 2\Delta\mu_{11}(\mathbf{k})\tau - \Delta\mu_{12}^*(\mathbf{k}), \qquad (7)$$

where $\mathbf{k} = \mathbf{k}[t,\varepsilon]$: see Appendix B. The solution of this equation can be represented in the form:

$$\tau(t) \approx Ce^{-i\varphi(t)} + \Delta\tau(t), \qquad (8)$$

where the first term is the solution of Eq. (7) at $\Delta\mu_{\rho\rho'} = 0$; C is some complex constant which should be found from the boundary condition (A.3); $\Delta\tau$ is a small correction proportional to $\Delta\mu_{\rho\rho'}$, and

$$\varphi(t) = 2\frac{\lambda|e|H}{\hbar c}\int_0^t dt'\psi(\mathbf{k}[t',\varepsilon]). \qquad (8)$$

Inserting $\tau(t)$ thus obtained into Eq. (A.4), we eventually arrive at

$$\Delta g \equiv g(\varepsilon, k_H) - g^{(0)}(\varepsilon^{(0)}, k_H) =$$

$$= \frac{m}{m^*}\frac{\Delta\varphi}{\pi} + \frac{4m}{\hbar}[\overline{\Delta\mu_{11}} + \mathrm{Re}\,(\overline{\Delta\mu_{12}C})], \qquad (9)$$

where the first term is due to the deformation of the electron orbit [i.e., it is caused by $\Delta\varepsilon(\mathbf{k})$,

$$\Delta\varphi \equiv \varphi(T) - \varphi^{(0)}(T),$$

the function $\varphi^{(0)}(T)$ is given by formula (8), but with $\mathbf{k}[t',\varepsilon]$ replaced by $\mathbf{k}^{(0)}[t',\varepsilon^{(0)}]$ in the argument of ψ (note that according to Eq. (A.7), one has $m\varphi^{(0)}(T)/(\pi m^*) = g^{(0)}$); the over $\Delta\mu_{\rho\rho'}$ means time averaging over the period T:

$$\overline{\Delta\mu_{\rho\rho'}} = \frac{1}{T}\int_0^T dt'\,\Delta\mu_{\rho\rho'}(\mathbf{k}^{(0)}[t',\varepsilon^{(0)}])\,e^{i\varphi^{(0)}(t)(\rho-\rho')},$$

and the constant C is determined from the equation,

$$\overline{\Delta\mu_{12}}C^2 + 2\left(\overline{\Delta\mu_{11}} + i\hbar\frac{1-e^{i\varphi(T)}}{2\pi m^*}\right)C - (\overline{\Delta\mu_{12}})^* = 0. \qquad (10)$$

It should be also emphasized that we are finding the difference in the g factors calculated at different energies ε and $\varepsilon^{(0)}$. However, since the difference $\varepsilon - \varepsilon^{(0)}$ is small, Appendix B, and we calculate Δg in the first order in $\Delta\varepsilon(\mathbf{k})$, $\Delta\mu_{\rho\rho'}(\mathbf{k})$, one may neglect the difference between ε and $\varepsilon^{(0)}$ in Eq. (9).

In the case of the one-band model, Appendix A, the function $\psi \equiv 1$, and thus $\Delta\varphi \equiv 0$. This means that in this case the Δg is determined only by $\Delta\mu_{\rho\rho'}$ rather than by $\Delta\varepsilon(\mathbf{k})$. Moreover, if the combination $\delta^{(0)} \equiv g^{(0)}m^*/4m$ is not close to an integer or a half-integer (i.e., the appropriate difference considerably exceeds $m^*|\overline{\Delta\mu_{12}}|/\hbar$), the constant C is relatively small, and the third term in Eq. (9) may be omitted. Then we arrive at symple formula:

$$\Delta g = \frac{4m\overline{\Delta\mu_{11}}}{\hbar}. \qquad (11)$$

In the case of the two-band model, Appendix A, the Δg depends both on the $\Delta\mu_{\rho\rho'}$ and on the $\Delta\varepsilon(\mathbf{k})$. Besides this, since in this case the electron energy levels in the magnetic field are doubly degenerate ($\delta^{(0)} = \pm 1/2$), the constant C is not small, and it follows from Eqs. (9), (10) that

$$\Delta g = \sqrt{\left(\frac{m}{m^*}\frac{\Delta\varphi}{\pi} + \frac{4m\overline{\Delta\mu_{11}}}{\hbar}\right)^2 + \left|\frac{4m\overline{\Delta\mu_{12}}}{\hbar}\right|^2}. \qquad (12)$$

3. Semiconductors

To apply our results to semiconductors, let us consider more closely the case of the one-band model of the electron energy spectrum, Eq. (2). Assuming that the energy is measured from the band edge $\varepsilon(\mathbf{k}_{ex})$ and the wave vector $\mathbf{k}$ from $\mathbf{k}_{ex}$, equation (2) is rewritten as follows:

$$\varepsilon^{(0)}(\mathbf{k}) = \sum_{\alpha=x,y,z} \hbar^2 k_\alpha^2 (2m_\alpha)^{-1}, \qquad (13)$$

where k_α are the components of $\mathbf{k}$. As was mentioned above, in the one-band case the correction Δg depends only on $\Delta\mu_{\rho\rho'}$ rather than on the correction to the energy dispersion relation, $\Delta\varepsilon$. Thus, it is sufficient to consider only $\Delta\mu_{\rho\rho'}$ here. Since $\mu_{\rho\rho'}^{(0)}$ is the constant matrix, Appendix A, the first correction to it is proportional to $\mathbf{k}$. However, this linear correction may be identically equal to zero due to symmetry of the crystal, and so we shall treat both the linear and the quadratic corrections to $\mu_{\rho\rho'}^{(0)}$:

$$\mu(\mathbf{k}) = \hat{c} + \sum_{\alpha=x,y,z} \hat{b}^\alpha k_\alpha + \sum_{\alpha,\beta=x,y,z} \hat{a}^{\alpha\beta} k_\alpha k_\beta, \quad (14)$$

where $\hat{c} \equiv \hat{\mu}^{(0)}$, and $\hat{b}^\alpha$, $\hat{a}^{\alpha\beta}$ are some constant matrices. The matrices $\hat{\mu}^{(0)}$, $\hat{b}^\alpha$, $\hat{a}^{\alpha\beta}$ depend only on the unit vector $\mathbf{n} \equiv \mathbf{H}/H$.

It should be also noted that formula (11) was derived in the representation in which the matrix c is diagonal. If this matrix is not assumed to be diagonal, formula (11) transforms into

$$\Delta g = \frac{4m}{\hbar T} \int_0^T dt \frac{c_{11}\Delta\mu_{11} + \mathrm{Re}\,(c_{12}^*\Delta\mu_{12})}{\lambda}, \quad (15)$$

where $\lambda = \sqrt{c_{11}^2 + |c_{12}|^2} = \sqrt{-\mathrm{Det}\,(\hat{c})}$. Using Eqs. (15) and (14), we find that

$$\Delta g = \frac{2m}{\hbar\lambda}\left(a_s\left[\frac{m_n\varepsilon}{\hbar^2} - \frac{k_H^2}{2}\right] + b_n k_H + a_n k_H^2\right), \quad (16)$$

where $k_H = \mathbf{n}\cdot\mathbf{k}$; $\mathbf{n} = \mathbf{H}/H$, and the $\mathbf{n}$-dependent parameters m_n, b_n, a_n, a_s are expressed via traces of the matrices $\hat{c}, \hat{b}^\alpha, \hat{a}^{\alpha\beta}$ as follows:

$$m_n = \sum_{\alpha=x,y,z} m_\alpha n_\alpha^2,$$

$$b_n = m_n^{-1}\sum_{\alpha=x,y,z} n_\alpha m_\alpha \mathrm{Tr}\,(\hat{c}\hat{b}^\alpha),$$

$$a_n = m_n^{-2}\sum_{\alpha,\beta=x,y,z} n_\alpha n_\beta m_\alpha m_\beta \mathrm{Tr}\,(\hat{c}\hat{a}^{\alpha\beta}),$$

$$a_s = m_n^{-1}\sum_{\alpha=x,y,z} m_\alpha \mathrm{Tr}(\hat{c}\hat{a}^{\alpha\alpha}) - a_n.$$

Experimental investigations of the oscillation effects enable one to measure the g factors of the electron orbits lying in the extremal cross sections of the Fermi surface (with respect to k_H) [1]. For spectrum (13) the extremal cross sections correspond to $k_H = 0$, and for such orbits we obtain from Eq. (16)

$$\Delta g(\varepsilon, k_H = 0) = \varepsilon \frac{2mm_n}{\hbar^3\lambda} a_s. \qquad (17)$$

Formulas (16) and (17) are the main result of this section. For a given matrix $\Delta\mu_{\rho\rho'}(\mathbf{k}, \mathbf{n})$ they enable one to find Δg *explicitly* for various ε, k_H, and directions of the magnetic field $\mathbf{n}$. However, these formulas fail for those $\delta^{(0)} \equiv g^{(0)}m^*/4m$ such that $\sin(2\pi\delta^{(0)}) \approx 0$; see Sec. 2. A more accurate estimate of the condition under which Eqs. (16) and (17) hold true yields

$$\left|\frac{\sin(2\pi\delta^{(0)})}{2\pi}\right| \gg \left|\frac{\Delta g m^*}{4m}\right|.$$

Note that the intervals of $\delta^{(0)}$ where Eqs. (16), (17) fail are very narrow when Δg is small.

4. Examples

III−V semiconductors

As an example, consider III−V semiconductors, and in particular, the well-known GaAs, which are widely used in practice. The semiconductors of this class have the zinc-blende crystal structure with the point of the band extremum, k_{ex}, being in the center of the Brillouin zone, i.e., $k_{ex} = 0$. These semiconductors have no center of inversion, and strictly speaking, the electron energy levels in these crystals do not degenerate in sspin even without a magnetic field. However, near the center of the Brillouin zone this splitting of the electron energy levels caused by the spin−orbit interaction is considerably less [40] than the splitting $\Delta E = g(e\hbar/2mc)H$ caused by the magnetic field that is usually applied to the samples in experiments. In this context the concept of the g factor is justified and is commonly used to describe the electron energy levels in magnetic field for III−V semiconductors.

The correction Δg has been investigated experimentally in these semiconductors, and it was found that [34]

$$\Delta g(\varepsilon) = \beta\varepsilon \qquad (19)$$

for the extremal cross sections ($k_H = 0$). The coefficient β varies from 144 eV^{-1} for InSb to 2.2 eV^{-1} for InP. Note that relation (19), found experimentally, is in complete agrement with our result, Eq. (17).

Let us take the axes of the coordinate system along the principal crystal axes. Then the energy dispersion

relation for these compounds has the form of Eq. (13) with $m_1 = m_2 = m_3 = m*$, while the matrix $\hat{\mu}(\mathbf{k}, \mathbf{n})$ can be written as [40,41]

$$\frac{e}{c}\hat{\mu}(\mathbf{k}, \mathbf{n}) = \frac{g^{(0)}}{2}\mu_B(\hat{\sigma}\mathbf{n}) + a_4\mathbf{k}^2(\hat{\sigma}\mathbf{n}) + 2a_5(\hat{\sigma}\mathbf{k})(\mathbf{kn}) +$$

$$+ a_6(\hat{\sigma}_x k_x^2 n_x + \hat{\sigma}_y k_y^2 n_y + \hat{\sigma}_z k_z^2 n_z), \quad (20)$$

where $\mathbf{n} = \mathbf{H}/H$, μ_B is the Bohr magneton, $g^{(0)}$ is the g factor at the band edge, and a_4, a_5, a_6 are some constant real parameters (expressions for these parameters in terms of the band-structure parameters can be found in Ref. 41). The first term in this expression describes $\hat{\mu}^{(0)} = c$ [see Eqs. (6), (14)], while the other terms in Eq. (20) give $\Delta\mu_{\rho\rho'}$. Note that the term linear in $\mathbf{k}$ is absent. Inserting these $\Delta\mu_{\rho\rho'}$ into formula (16), we immediately arrive at

$$\Delta g(\varepsilon, k_H) = \frac{8mm*c}{\hbar^3|e|}\left[a_4\varepsilon + 2a_5\frac{\hbar^2 k_H^2}{2m*} + \right.$$

$$\left. + a_6\left(\varepsilon F(\theta,\varphi) + \frac{\hbar^2 k_H^2}{2m*}(1 - 3F(\theta,\varphi))\right)\right], \quad (21)$$

where

$$F(\theta,\varphi) = \frac{1}{2}\left(1 - \sum_{\alpha = x,y,z} n_\alpha^4\right) =$$

$$= \sin^2\theta\,(\sin^2\theta\cos^2\varphi\sin^2\varphi + \cos^2\theta),$$

and the angles θ and φ are defined as follows:

$$\mathbf{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta). \quad (22)$$

Expression (21) completely agrees with that calculated in Ref. 40. At $k_H = 0$, formula (21) yields

$$\Delta g(\varepsilon) = \frac{8mm*c\varepsilon}{|e|\hbar^3}(a_4 + a_6 F(\theta,\varphi)),$$

i.e., we obtain the expression for the coefficient β in relation (19). For the case $\varphi = \pi/4$ formula (22) coincides with that derived in Ref. 41 by another method, and it very well describes the experimental angular dependences of Δg for GaAs [42].

According to Ref. 34, one has $g^{(0)} = -0.44$ and $\beta \approx 6.3 \text{ eV}^{-1}$ for GaAs. But it is well known that even a small amount of Al significantly shifts $g^{(0)}$ to positive values. This property of the compound $Al_x Ga_{1-x}As$ is now used in the spintronic devices [43]. At a concentration $x \approx 0.1$ the electron g factor $g^{(0)} \approx 0$. Then condition (18) fails, and Eq. (9) must be used to calculate Δg. Eventually, in the region of concentrations x where $g^{(0)} \approx 0$, we obtain

$$\Delta g = \frac{8mm*c\varepsilon}{\hbar^3|e|}\sqrt{[a_4 + a_6 F(\theta,\varphi)]^2 + a_6^2 G(\theta,\varphi)}, \quad (23)$$

where

$$G(\theta,\varphi) = \frac{\sin^6\theta}{64}[\cos^2\theta(\cos 4\varphi + 7) + \sin^2 4\varphi].$$

Note that the angular dependence of Δg described by Eq. (23) differs noticeably from that given by Eq. (22).

Bismuth

In bismuth near the symmetry points L of its Brillouin zone there are two bands, $\varepsilon_0(\mathbf{k})$ and $\varepsilon_a(\mathbf{k})$, which are close to each other and to the Fermi energy [1,35]. (These bands which we denote by subscripts 0 and a are separated by a gap $E_g = \varepsilon_0 - \varepsilon_a \sim 10$ meV at this point.) The electron Fermi surface of Bi consists of three «ellipsoids» located near the three points L. The symmetry of this point is C_{2h}. It is common practice to put the origin of the coordinate system (i.e., the point $\mathbf{k} = 0$) at L, to take the x axis along the twofold axis C_2, to place the yz plane on the reflection plane σ_h, and to choose the y axis in the direction of the longest principal axis of the ellipsoid (this axis is approximately ten times longer than the other two). Since the Fermi surface of bismuth is elongated in the k_y direction, the two-band model is not sufficient to describe the electron energy spectrum in this direction, and the following extended two-band model of McClure [44,45] is commonly used:

$$\left[\frac{\varepsilon - (\alpha_0 - \alpha_a)k_y^2}{4}\right]^2 = \left[\frac{E_g}{2} + \frac{(\alpha_0 + \alpha_a)k_y^2}{4}\right]^2 +$$

$$+ q_1^2 k_x^2 + |q_2|^2 k_y^2 + q_3^2 k_z^2, \quad (24)$$

where the energy ε is measured from the middle of the energy gap E_g at the point L; α_0, α_a, q_1 and q_3 are real parameters of the model, while q_2 is an imaginary constant, $\text{Re}(q_2) = 0$. The values of all these parameters are well known [46,47]. It is essential that the value of $|q_2|$ is relatively small. It is for this reason that the Fermi surface is elongated in the k_y direction, and the terms $\alpha_0 k_y^2$, $\alpha_a k_y^2$ are taken into account. Without these terms, Eq. (24) reduces to the two-band model.

The g factors of the central cross sections of the Fermi surface of Bi have been measured with high accuracy [35]. When the magnetic field is directed along y, one has $k_y = 0$ for the central cross section, and Eq. (24) reduces to the two-band model. This model sufficiently well describes the spectrum of bismuth in this situation, and hence $\delta \equiv gm*/4m \approx 1/2$. If the magnetic fields deviates from the y axis, a correction to

this two-band result appears, and this correction was calculated in Ref. 28 for an arbitrary angle between **H** and the y axis. Here we shall consider the terms with α_0, α_a as small corrections and shall find Δg for the conduction band $\varepsilon_0(\mathbf{k})$, using Eq. (12). It is clear that this approach is valid at sufficiently small angles η between **H** and the y axis.

It follows from Eq. (24) that

$$\varepsilon_0(\mathbf{k}) = \varepsilon_0^{(0)}(\mathbf{k}) + \Delta\varepsilon,$$

$$\varepsilon_0^{(0)}(\mathbf{k}) = \sqrt{(E_g/2)^2 + q_1^2 k_x^2 + |q_2|^2 k_y^2 + q_3^2 k_z^2},$$

$$\Delta\varepsilon = \frac{(\alpha_0 - \alpha_a)k_y^2}{4} + \frac{E_g}{2\varepsilon_0^{(0)}(\mathbf{k})}\frac{(\alpha_0 + \alpha_a)k_y^2}{4}.$$

The matrix elements of $\hat{\mu}_0$ for the central cross sections of the Fermi surface of Bi were calculated in Ref. 28. They are

$$\mu_{0,11}(\varepsilon) \equiv \mu_{11}^{(0)} + \Delta\mu_{11} = A[-iBq_2q_3n_x +$$

$$+ \tilde{\rho}_0(E_a - \varepsilon)^2 + \tilde{\rho}_a(t^2 - |u|^2) + t(\tilde{\nu}_a u^* + \tilde{\nu}_a^* u)], \quad (25)$$

$$\mu_{0,12}(\varepsilon) \equiv \mu_{12}^{(0)} + \Delta\mu_{12} = A[iBq_1(q_3n_y - q_2n_z) -$$

$$-2\tilde{\rho}_a tu + \tilde{\nu}_0(E_a - \varepsilon)^2 + \tilde{\nu}_a t^2 - \tilde{\nu}_a^* u^2], \quad (26)$$

where

$$A = [(E_a - \varepsilon)(E_0 + E_a - 2\varepsilon)]^{-1};$$

$$B = (E_a + E_g + \varepsilon)/\hbar; \quad E_{0,a}(\mathbf{k}) = \pm\left(\frac{E_g}{2} + \frac{\alpha_{0,a}}{2}k_y^2\right);$$

$$t = q_1k_x; \quad u = q_2k_y + q_3k_z,$$

and

$$\tilde{\rho}_{0,a} = \rho_{0,a}n_x, \tilde{\nu}_{0,a} = \nu_{0,a}^y n_y + \nu_{0,a}^z n_z.$$

Here n_i are the components of the vector $\mathbf{n} = \mathbf{H}/H$; ρ_0, ρ_a are some real constants, and ν_0^y, ν_a^y, ν_0^z, ν_a^z are constant complex parameters. The matrix $\hat{\mu}_0^{(0)}$ is obtained from Eqs. (25), (26) by setting $\rho_{0,a} = \nu_{0,a}^y = \nu_{0,a}^z = \alpha_{0,a} = 0$. Note that Eqs. (25), (26) take into account corrections to the two-band model even for magnetic field directed along the y axis $(n_x = n_z = 0)$.

Using Eq. (12), we obtain

$$\delta \approx \frac{1}{2} + \frac{\varepsilon}{2\Lambda}\left[h|q_2|q_3n_x^2\bar{\rho} + \frac{1}{8}(q_1^2n_z^2 + q_3^2n_x^2)\left(1 - \frac{E_g}{2\varepsilon}\right)\bar{\alpha} +\right.$$

$$\left. + hq_1 \operatorname{Im}([q_3n_y + i|q_2|n_z][\bar{\nu}^y n_y + \bar{\nu}^z n_z])\right],$$

$$(27)$$

where

$$\Lambda = n_y^2 q_1^2 q_3^2 + n_z^2 q_1^2|q_2|^2 + n_x^2|q_2|^2 q_3^2,$$

$$\bar{\rho} = \rho_a\left[1 - \frac{E_g}{2\varepsilon}\right] - \rho_0\left[1 + \frac{E_g}{2\varepsilon}\right],$$

$$\bar{\nu}^\beta = \nu_a^\beta\left[1 - \frac{E_g}{2\varepsilon}\right] + \nu_0^\beta\left[1 + \frac{E_g}{2\varepsilon}\right],$$

$$\bar{\alpha} = \alpha_0\left[1 + \frac{E_g}{2\varepsilon}\right] - \alpha_a\left[5 + \frac{E_g}{2\varepsilon}\right],$$

with $\beta = y$, z. Formula (27) can be further symplified if one takes into account that this expression is valid only for $n_y \neq 0$ and that the ratio $(|q_2|^2/q_1q_3)$ is of the order of 10^{-2} in bismuth [46,47]. Then, we may put $\Lambda \approx n_y^2 q_1^2 q_3^2$, and eventually we find

$$\delta \approx \delta(0) + C_1 \tan\eta \cos\zeta +$$

$$+ \tan^2\eta\, [C_{2x}\sin^2\zeta + C_{2z}\cos^2\zeta], \quad (28)$$

where the following parametrization for the vector $\mathbf{n} \equiv \mathbf{H}/H$ has been used: $\mathbf{n} = (\sin\eta\sin\zeta, \cos\eta, \sin\eta\cos\zeta)$. The quantity $\delta(0)$ is the value of δ for magnetic field directed along y, i.e., when the angle η between **H** and this axis is zero. Note that this $\delta(0)$ differs from $1/2$ if the parameter $\bar{\nu}^y$ has an imaginary part,

$$\delta(0) = \frac{1}{2} + \frac{\hbar\varepsilon}{2q_1q_3}\operatorname{Im}\bar{\nu}^y.$$

The constants C_1, C_{2x}, C_{2z} are

$$C_1 = \frac{\hbar\varepsilon}{2q_1q_3^2}(q_3\operatorname{Im}\bar{\nu}^z + |q_2|\operatorname{Re}\bar{\nu}^y),$$

$$C_{2x} = \frac{\hbar\varepsilon|q_2|}{2q_1^2q_3}\bar{\rho} + \frac{\varepsilon - E_g/2}{16q_1^2}\bar{\alpha},$$

$$C_{2z} = \frac{\hbar\varepsilon|q_2|}{2q_1q_3^2}\operatorname{Re}\bar{\nu}^z + \frac{\varepsilon - E_g/2}{16q_3^2}\bar{\alpha}$$

It is clear from these formulas that an experimental investigation of angular dependences of δ in the xy and yz planes (i.e., in the planes $\zeta = \pi/2$ and $\zeta = 0$) near the y direction would enable one to measure $\delta(0)$, C_1, C_{2x}, C_{2z} and hence to extract the parameters $\operatorname{Im}\bar{\nu}^y$, $q_3\operatorname{Im}\bar{\nu}^z + |q_2|\operatorname{Re}\bar{\nu}^y$, $\operatorname{Re}\bar{\nu}^z$, and $\bar{\rho}$ from the appropriate experimental data.

In Fig. 1 we compare the δ obtained using the *explicit* formula (28) with the δ calculated *numerically* in Ref. 28. Note that in Ref. 28 the terms $\alpha_0 k_y^2$, $\alpha_a k_y^2$ were not assumed to be small, and hence the results for δ are valid even at $\eta \sim \pi/2$. Interestingly, the approximate formula (28) describes δ quantitatively even if the vector **n** substantially deviates from the y axis.
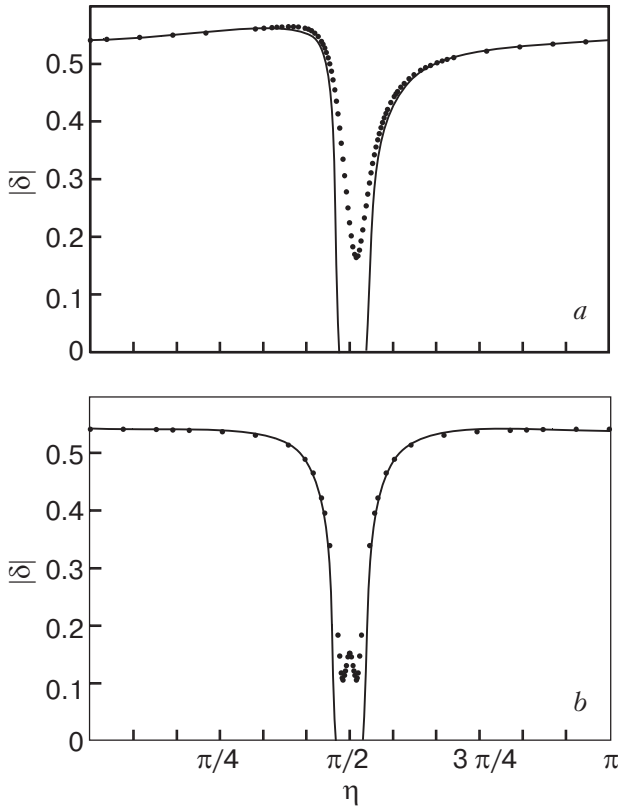
Fig. 1. The dependence of $\delta \equiv gm^*/4m$ on the magnetic-field direction in Bi, Eq. (28), (solid lines). The values of the parameters are the same as in Ref. 28. The magnetic field lies either in the yz plane (a) or in the xy plane (b). The angle η is measured from the y axis; the positive direction of y is taken as in Ref. 35. The dotted lines show the appropriate results of Ref. 28, which well describe the experimental data [35].

Appendix A: formulas for the g factor

Here we present the equations determining the g factor [5,8] and the solutions of these equations [28] for the cases of the one-band and two-band models of the electron energy spectrum.

As is well known [4], in the semiclassical approximation an electron in a crystal in a magnetic field $\mathbf{H}$ may be considered as a wave packet, with the wave vector of the packet $\mathbf{k}$ moving in an orbit [7] Γ in the Brillouin zone. The dependence of the wave vector $\mathbf{k}$ on the time t can be found from the equation,

$$\hbar \dot{\mathbf{k}} = \frac{|e|}{c}[\mathbf{H} \times \mathbf{v}(\mathbf{k})], \qquad (A.1)$$

where the electron velocity is given by

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon(\mathbf{k})}{\partial \mathbf{k}}.$$

During the electron motion in the orbit Γ, the direction of its spin $\mathbf{s}$ changes due to the spin−orbit interaction. To describe the direction of the electron spin in the semiclassical approximation, we introduce the complex parameter $\tau(\mathbf{k})$ that defines the components of the electron wave function $\Psi(\mathbf{k})$ in the spinor space of the Hamiltonian (4) as follows:

$$\Psi(\mathbf{k}) \propto \begin{pmatrix} 1 \\ \tau \end{pmatrix}.$$

This definition leads to the following representation of the electron spin at the point $\mathbf{k}$ of the semiclassical orbit:

$$\mathbf{s} = \frac{1}{2}\frac{(2\mathrm{Re}\tau,\, 2\mathrm{Im}\tau,\, 1-|\tau|^2)}{1+|\tau|^2}.$$

Then, the dynamics of the electron spin may be described by a function $\tau(t)$. This function obeys the equation: [5,8]

$$i\hbar\dot{\tau} = \frac{|e|H}{c}(\mu_{12}\tau^2 + 2\mu_{11}\tau - \mu_{12}^*). \qquad (A.2)$$

Here $\mu_{\rho\rho'} = \mu_{\rho\rho'}[\mathbf{k}(t)]$ are the matrix elements of the matrix $\hat{\mu}$ in Eq. (4), and $\mathbf{k}(t)$ is the function determined from Eq. (A.1). The boundary condition to Eq. (A.2) is

$$\tau(T) = \tau(0), \qquad (A.3)$$

where $T = 2\pi cm^*/(|e|H)$ is the period of the electron motion in the orbit Γ, and m^* is the electron cyclotron mass.

On calculating the functions $\mathbf{k}(t)$ and $\tau(t)$, the electron g factor for a closed orbit Γ is given by [5,8]

$$g = -\frac{2m|e|H}{\pi m^*\hbar c}\int_0^T dt\left(\mu_{11}(\mathbf{k}) + \mathrm{Re}\left\{\tau(t)\mu_{12}(\mathbf{k})\right\}\right) \quad (A.4)$$

Here $\mathbf{k}$ denotes the function $\mathbf{k}(t)$ determined from Eq. (A.1). Since the combination $|e|Hdt/c$ is proportional to the infinitesymal element $|d\mathbf{k}|$ of the orbit Γ, see Eq. (A.1), the appearance of the factor $|e|H/c$ in Eq. (A.4), of course, does not mean the proportionality of g to H. This factor is due only to the parametrization of the electron orbit with the use of the time t.

For the one-band and two-band models of the electron energy spectrum, the orbit Γ is an ellipse, and the function $\mathbf{k}(t)$ is easily found from Eq. (A.1). In both these cases the matrix $\mu_{\rho\rho'}$ has the form [28]

$$\mu_{\rho\rho'}^{(0)}(\mathbf{k}) = \psi(\mathbf{k})c_{\rho\rho'}, \qquad (A.5)$$

where $\rho, \rho' = 1, 2$, $\psi(\mathbf{k})$ is some real function of the wave vector (and of the electron energy), and $c_{11} = -c_{22}$ and $c_{12} = c_{21}^*$ are real and complex constants, respectively. Using Eq. (A.5), equation (A.2) with boundary condition (A.3) is solved exactly,

$$\tau = (-c_{11} \pm \lambda) / c_{12},$$

where

$$\lambda = \sqrt{(c_{11})^2 + |c_{12}|^2}. \qquad (A.6)$$

Then, it follows from Eq. (A.4) that the g factor for these models is

$$g^{(0)} = \pm \frac{2m\lambda |e| H}{\pi m^* \hbar c} \int_0^T dt \psi(\mathbf{k}(t)). \qquad (A.7)$$

In the one-band case one has [28] $\psi = 1$, $c_{\rho\rho'} = \mu_{\rho\rho'}(\mathbf{k}_{ex})$, where $\mathbf{k}_{ex}$ is the point of the band extremum in the Brillouin zone. Using the formula $T = 2\pi c m^* / (|e| H)$, we obtain,

$$g^{(0)} = \pm 4m\lambda/\hbar.$$

Note that in the one-band model this $g^{(0)}$ does not depend on the energy and thus coincides with the g factor at the band edge.

In the two-band case one has [28]

$$\psi(\mathbf{k}) = \frac{\hbar [\varepsilon + 0.5E_g - \hbar \mathbf{v}_a(0)\mathbf{k}]^{-1}}{2\varepsilon - \hbar[\mathbf{v}_0(0) - \mathbf{v}_a(0)]\mathbf{k}},$$

where ε is the electron energy, and the other notations are as in Eq. (3). The explicit expressions for $c_{\rho\rho'}$ are presented in Ref. 28. Integrating Eq. (A.7), we now arrive at [28]

$$g^{(0)} = \pm 2m/m^*.$$

Note that in this case the combination $\delta \equiv gm^*/(4m)$ is equal to $\pm 1/2$, and thus the electron energy levels in the magnetic field are doubly degenerate [29].

Appendix B: deformation of the electron orbit

An electron moving in the semiclassical orbit in a magnetic field has a constant energy ε. Suppose that the solution of Eq. (A.1) for the dispersion relation $\varepsilon^{(0)}(\mathbf{k})$ is known, and that the electron orbit at the energy $\varepsilon^{(0)}$ is given by some function $\mathbf{k}^{(0)}[t, \varepsilon^{(0)}]$. We now find the new orbit

$$\mathbf{k}[t, \varepsilon] = \mathbf{k}^{(0)}[t, \varepsilon^{(0)}] + \Delta\mathbf{k}[t].$$

which corresponds to the new energy ε and to the modified dispersion relation (5). We obtain

$$\Delta\mathbf{k}(t) = \mathbf{F}_{\parallel}(\mathbf{k}^{(0)}(t)) + [\mathbf{n} \times \mathbf{v}_{\perp}^{(0)}] \times$$

$$\times \left\{ F(t) - \frac{\int_0^T dt' (\mathbf{v}_{\perp}^{(0)}(t'))^2 F(t')}{\int_0^T dt' (\mathbf{v}_{\perp}^{(0)}(t'))^2} \right\},$$

where $\mathbf{n} \equiv \mathbf{H}/H$, and $\mathbf{v}_{\perp}^{(0)}$ is the component of the velocity $\mathbf{v}^{(0)} \equiv (1/\hbar)(\partial \varepsilon^{(0)}(\mathbf{k})/\partial \mathbf{k})$ perpendicular to the magnetic field,

$$F(t) = \int_0^t dt' \frac{eH}{c\hbar} [\nabla_{\mathbf{k}_{\perp}} \mathbf{F}_{\parallel}(\mathbf{k})] \big|_{\mathbf{k} \to \mathbf{k}^{(0)}(t')},$$

and

$$\mathbf{F}_{\parallel}(\mathbf{k}) = \frac{[\varepsilon - \varepsilon^{(0)} - \Delta\varepsilon(\mathbf{k})] \mathbf{v}_{\perp}^{(0)}(\mathbf{k})}{\hbar [\mathbf{v}_{\perp}^{(0)}(\mathbf{k})]^2}.$$

In calculating the change of the g factor, Δg, it is convenient to chose the constant $\varepsilon^{(0)}$ so that the periods of the electron motion (and hence the cyclotron masses) are the same for the orbits $\mathbf{k}[t, \varepsilon]$ and $\mathbf{k}^{(0)}[t, \varepsilon^{(0)}]$, i.e.,

$$\Delta T \equiv T - T^{(0)} = \int_0^T dt' (\nabla_{\mathbf{k}_{\perp}} \mathbf{F}_{\parallel}(\mathbf{k})) \big|_{\mathbf{k} \to \mathbf{k}^{(0)}(t')} =$$

$$= \frac{c\hbar}{eH} F(T) = 0.$$

This condition is assumed to be fulfilled throughout this paper.

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