Calculation of conduction electron *g* factor in metals: Comparison of electron-spin dynamics and local *g*-factor approaches

G. P. Mikitik and Yu. V. Sharlai
B. Verkin Institute For Low Temperature Physics and Engineering, National Ukrainian Academy of Sciences, Kharkov 61103, Ukraine
(Received 6 November 2002; revised manuscript received 3 January 2003; published 19 March 2003)

We analyze and compare two approaches to calculations of the *g* factors of electron semiclassical orbits in metals. The first, exact approach takes into account a dynamics of the electron spin when the Bloch electron moves in a magnetic field. The second, more simple approach is based on the concept of the so-called local *g* factor and completely neglects this dynamics. It is pointed out that the second approach is approximately valid not only at a weak spin-orbit interaction in crystals but also at an arbitrary strength of this interaction if the Fermi level of electrons lies near an edge of the electron energy band under consideration or if the electron spectrum specifying the semiclassical orbit can be well described by a two-band model. As an example of the spectrum with more than two bands and with the strong spin-orbit interaction, we consider the electron spectrum of bismuth when the direction of the magnetic field is close to the trigonal-binary plane of the crystal and calculate the *g* factors of the appropriate electron orbits.

DOI: 10.1103/PhysRevB.67.115114 PACS number(s): 71.18.+y, 71.70.Di, 71.70.Ej

I. INTRODUCTION

As known well,[1] the *g* factor of conduction electrons in metals *g* specifies the splitting of the 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, *H* is the external magnetic field, and the crystal is implied to have a center of inversion (and only such crystals are considered below). In this paper we shall discuss the *g* factors which are experimentally found from oscillation effects in the semiclassical limit when there are a lot of the Landau levels under the Fermi surface of the metal. Besides this, we do not consider the situations when the magnetic breakdown occurs. As well known,[2] in this case an electron in the crystal in a magnetic field may be considered as a wave packet, with the wave vector of the packet $\mathbf{k}$ moving in a semiclassical orbit Γ in the Brillouin zone. The orbit is the intersection of the constant-energy surface of the electron in the absence of the magnetic field, $\varepsilon(\mathbf{k})$ is equal to a const, with the plane k_H is equal to a const, where k_H is the component of the wave vector in the direction of the external magnetic field $\mathbf{H}$. In this approach the semiclassical *g* factor appears in the well-known quantization rule[1,3,4] for electron energy ε in a magnetic field

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

where *S* is the cross-sectional area of the *closed* orbit Γ, *n* is a large integer, the cyclotron mass $m^*=(\hbar^2/2\pi)(\partial S(\varepsilon,k_z)/\partial\varepsilon)$, 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 a location of the *orbit* Γ in the Brillouin zone.

Calculations of the *g* factors were carried out for various metals.[9–29] It is necessary to stress that all these calculations were based on the concept of the so-called local *g* factor $g(\mathbf{k})$. This concept was introduced in Ref. 30 to describe the *g* factors for *points* $\mathbf{k}$ on the Fermi surface, and in the above-mentioned publications the *g* factor for the orbit Γ was obtained by the averaging of $g(\mathbf{k})$ over this Γ. However, as it follows from Refs. 7 and 8, only the *g* factors of closed *orbits* have a strict physical meaning, while the concept of the local *g*-factor can be applied only approximately when a strength of the spin-orbit interaction in the metal is sufficiently weak.[8] The exact formulas for the *g* factor[7,8] are applicable at any strength of the spin-orbit coupling, but they are more complicated than in the local *g*-factor approach. In this paper, we consider various types of the electron energy-band structure in crystals and point out situations, for which one may expect an essential difference in results obtained in the framework of the exact approach and of the approach based on the concept of the local *g* factor. Since the electron spectrum of bismuth provides an example of such a situation, we analyze the *g* factors of extremal orbits lying on the electron ellipsoids of the Fermi surface of bismuth and show that for directions of the magnetic field near the plane containing the trigonal and the binary axes, the exact *g* factors do noticeably differ from values derived on the basis of local *g*-factor approximation. We also demonstrate that the obtained results for the *g* factors well agree with the experimental data.[31]

The paper is organized as follows: In Sec. II, we briefly describe the theoretical results for the *g* factor. We also explain distinctions between the exact approach to the *g*-factor calculation and the local *g*-factor approximation, and point out situations for which the approaches may lead to different results. In Sec. III the necessary information on the electron-band structure of bismuth is presented, and the *g* factors of the orbits lying on the electron ellipsoids are calculated in the framework of both the approaches. We also compare the derived exact results for the *g* factor with the appropriate experimental data.[31] Some mathematical details of our analysis are presented in Appendices A and B.

II. TWO APPROACHES TO THE g FACTOR CALCULATIONS

A. Formulas for the g factor

The g factor in the quantization rule (1) can be expressed in terms of matrix elements of the effective one-band Hamiltonian $\hat{H}_{eff}$ of a Bloch electron in a magnetic field. Since electron bands are twofold degenerate in crystals with the inversion symmetry,[2] the Hamiltonian is a 2×2 matrix in a spinor space. According to Refs. 32 and 33, this Hamiltonian to first order in the magnetic field H has the form

$$\hat{\mathrm{H}}_{eff}=\varepsilon_0(\hat{\mathbf{k}})\hat{\mathbb{I}}+\frac{e}{c}H\hat{\mu}_0(\mathbf{k},\mathbf{n}), \tag{2}$$

where $\mathbf{n}$ is the unit vector directed along the magnetic field $\mathbf{H}$, $\varepsilon_0(\mathbf{k})$ is the electron dispersion relation for the band being investigated (from here on we denote this band by the subscript 0), $\hat{\mathbf{k}}=\mathbf{K}-(e/c\hbar)\mathbf{A}(i\partial/\partial\mathbf{K})$, $\mathbf{A}(\mathbf{r})$ is the vector potential of the magnetic field $\mathbf{H}$, and the function $\varepsilon_0(\hat{\mathbf{k}})$ in Eq. (2) is implied to be completely symmetrized in the components of $\hat{\mathbf{k}}$. Elements of the matrix $\hat{\mu}_0$ are the sums

$$\mu_{0,\rho\rho'}=\mu^{s}_{0,\rho\rho'}+\mu^{or}_{0,\rho\rho'},$$

of the pure spin parts $\mu^{s}_{0,\rho\rho'}$

$$\mu^{s}_{0,\rho\rho'}(\mathbf{k})=-\frac{\hbar}{2m}\int_v u^{*}_{\mathbf{k},0\rho}(\mathbf{r})(\mathbf{n}\sigma)u_{\mathbf{k},0\rho'}(\mathbf{r})d\mathbf{r}, \tag{3}$$

and the orbital contributions $\mu^{or}_{0,\rho\rho'}$

$$\mu^{or}_{0,\rho\rho'}(\mathbf{k})=(\mathbf{n}[\mathbf{v}_0\times\mathbf{\Omega}_{0\rho,0\rho'}])+\frac{\hbar}{2i}\sum_{\rho'',m\neq 0}\frac{(\mathbf{n}[\mathbf{v}_{0\rho,m\rho''}\times\mathbf{v}_{m\rho'',0\rho'}])}{\varepsilon_m(\mathbf{k})-\varepsilon_0(\mathbf{k})}, \tag{4}$$

where the spin indexes $\rho,\rho',\rho''=1,2$; σ_i is the Pauli matrices; $\mathbf{v}_0=(1/\hbar)(\partial\varepsilon_0/\partial\mathbf{k})$; $\mathbf{v}_{n\rho,m\rho'}$ and $\mathbf{\Omega}_{n\rho,m\rho'}$ are the matrix elements of the velocity operator and the periodic in $\mathbf{k}$ part of the position operator

$$\mathbf{\Omega}_{n\rho,m\rho'}(\mathbf{k})=i\int_v u^{*}_{\mathbf{k},n\rho}(\mathbf{r})\frac{\partial}{\partial\mathbf{k}}u_{\mathbf{k},m\rho'}(\mathbf{r})d\mathbf{r}, \tag{5}$$

calculated in the $\mathbf{k}$ representation. In Eqs. (3) and (5) the integration is over a unit cell of the crystal lattice v, and $u_{\mathbf{k},l\rho}(\mathbf{r})$ is the periodic factor in the Bloch wave function of the lth band

$$\psi_{\mathbf{k},l\rho}=\exp(i\mathbf{kr})u_{\mathbf{k},l\rho}.$$

It is always assumed that $u_{\mathbf{k},l2}=(i\sigma_2 KI)u_{\mathbf{k},l1}$ where I, K, and $i\sigma_2 K$ are the spatial inversion, complex conjugation, and time reversal operators, respectively. With this choice of the spinors, the property $\mu_{0,11}=-\mu_{0,22}$ holds.[34] Several formulas simplifying calculations of $\mu_{0,\rho\rho'}$ in real situations were derived in the Appendix of Ref. 8 (see also Sec. II B and Appendix B below).

In 1969, De Graaf and Overhauser[30] introduced the concept of the local g factor associated with the *points* $\mathbf{k}$ of the Fermi surface of a metal. In our notations their quantity is described by the expression

$$g(\mathbf{k})=-(4m/\hbar)\mu_{0,11}(\mathbf{k}). \tag{6}$$

In this approach, the g factor of the orbit Γ is obtained by averaging $g(\mathbf{k})$ over Γ

$$g=\frac{\oint_\Gamma d\kappa g(\mathbf{k})/v_\perp}{\oint_\Gamma d\kappa/v_\perp}=\frac{2m}{\pi m^*}\oint_\Gamma\frac{d\kappa}{v_\perp}[-\mu_{0,11}(\mathbf{k})], \tag{7}$$

where $v_\perp$ is the absolute value of projection of $\mathbf{v}$ on the plane normal to $\mathbf{H}$; $d\kappa$ is the infinitesimal element of the orbit Γ, and we have inserted the well-known formula[2] for the cyclotron mass, $m^*=(\hbar/2\pi)\oint_\Gamma d\kappa/v_\perp$. It is Eq. (7) that was used in numerous publications.[9–29]

The exact expressions for the g factor in the semiclassical limit were derived in Refs. 7,5, and 8. In order to write these expressions, it is convenient to introduce the complex parameter $\tau(\mathbf{k})$ that defines the direction of the electron spin

$$\begin{pmatrix}1\\ \tau\end{pmatrix}$$

in the spinor space of the Hamiltonian (2) at the point $\mathbf{k}$ of the orbit Γ. Then, the g factor of the orbit Γ is given by[5,8]

$$g=-\frac{2m}{\pi m^*}\oint_\Gamma\frac{d\kappa}{v_\perp}\left[\mu_{0,11}+\frac{(\tau\mu_{0,12}+\tau^*\mu^*_{0,12})}{2}\right]. \tag{8}$$

The function $\tau(\mathbf{k})$ along the semiclassical orbit is specified by the equation

$$iv_\perp\frac{d\tau}{d\kappa}=\mu_{0,12}\tau^2+2\mu_{0,11}\tau-\mu^*_{0,12}, \tag{9}$$

with the boundary condition

$$\tau(0)=\tau(\kappa_0), \tag{10}$$

where τ is written as a function of a length along the electron trajectory and κ_0 is the perimeter of the orbit. Formulas (8), (9), and (10) permit one to find the g factor for any electron orbit.

Taking into account the well-known relation,[2] $(d\kappa/v_\perp)=(eH/c\hbar)dt$, Eq. (9) can be understood as the equation for spin dynamics of the electron moving in the semiclassical orbit (during the motion a direction of the electron spin changes due to the spin-orbit coupling). Then, boundary condition (10) simply means that in the steady state the direction of the electron spin must periodically return to its initial value.

It should be also emphasized that expression (8) generally does not admit defining the local g factor even though one finds the solution of Eqs. (9) and (10) and inserts this solution into Eq. (8). Indeed, the integrand of Eq. (8) at the point $\mathbf{k}$ depends on the electron states of the *whole* orbit Γ [τ at

the point $\mathbf{k}$ is determined by $\mu_{0,\rho\rho'}(\mathbf{k}')$ with $\mathbf{k}' \neq \mathbf{k}$, see Eq. (9)], so it cannot be considered as a local quantity which is determined only by the electron state corresponding to the point $\mathbf{k}$. Besides this, a true local g factor should be expressible through its values for three mutually orthogonal directions of the magnetic field. However, if one tilts the magnetic field and considers the point $\mathbf{k}_0$ on the Fermi surface which is the intersection point of the initial and the tilted orbits, the integrand of Eq. (8) at $\mathbf{k}_0$ generally does not satisfy this condition, since $\tau(\mathbf{k}_0)$ at different directions of $\mathbf{H}$ are determined by different orbits.

B. Comparison of the approaches

Since the g factor is the *measurable* quantity, formula (8) must be independent of a choice of the basis in the spinor space, i.e., must be invariant under unitary transformations in this space. The unitary transformations can be represented as a product of matrices corresponding to phase transformations of the Bloch factors $u_{\mathbf{k},l\rho}$ and to rotations in the space of these factors (see Appendix A). Equation (8) is invariant under the phase transformations.[8] In Appendix A we show that this equation is also invariant under the rotations. Thus, the exact formula for the g factor (8) really satisfies the abovementioned physical requirement.

Although formula (7) is invariant under the phase transformations, the rotations in the spinor space change its form, Appendix A. Thus, values of the g-factors determined by this expression depend on the basis in the spinor space used in calculations of the matrix $\hat{\mu}_0$, and formula (7) could be valid only in a specific basis. Although De Graaf and Overhauser did not point out this basis in their paper, it is easy to guess it. In this basis, the matrix $\hat{\mu}_0(\mathbf{k})$ should be diagonal at every point $\mathbf{k}$ of the Fermi surface. Then, one has $\mu_{0,12}(\mathbf{k})=0$; the solution of Eqs. (9) and (10) is $\tau=0$ for any orbit, and formulas (8) and (7) coincide. Note that just this basis was implied in the numerous publications mentioned above. However, in practice there exists a problem of determining this basis since under an unitary transformation $\hat{U}(\mathbf{k})$, the matrix $\hat{\mu}_0(\mathbf{k})$ changes as follows,

$$\hat{\mu}_0' = \hat{U}^+ \hat{\mu}_0 \hat{U} + i\left(\mathbf{n}\left[\mathbf{v}_0 \times \hat{U}^+ \left(\frac{\partial \hat{U}}{\partial \mathbf{k}} \right) \right] \right), \tag{11}$$

and the problem of calculating the appropriate $\hat{U}(\mathbf{k})$ [transforming $\hat{\mu}_0(\mathbf{k})$ to the diagonal form] is equivalent to that of solving Eqs. (9) and (10). In other words, in this way of the calculations, one deals with another representation of these equations, and formula (7) is the specific form of Eq. (8). In any other basis, Eq. (7) is not exact since De Graaf and Overhauser did not take into account the dynamics of the electron spin when they analyzed the semiclassical motion of the electron wave packet in the magnetic field.

Applicability of Eq. (7) in the specific basis does not mean that the local g-factor approach is true. This approach is valid if the dynamics of the electron spin is absent at all, i.e., if there exists a basis in the spinor space in which τ is a constant for *any* direction of the magnetic field (the value of the constant may depend on the direction of the magnetic field, $\mathbf{n}$). In this case the arguments of Sec. II A against the concept of the local g factor do not work, and Eq. (9) determines this τ through the elements of the matrix $\hat{\mu}_0$,

$$\tau = \frac{-\mu_{0,11} \pm \sqrt{(\mu_{0,11})^2 + |\mu_{0,12}|^2}}{\mu_{0,12}}. \tag{12}$$

It follows from this relation that for τ to be constant, the matrix $\hat{\mu}_0$ must have the form

$$\hat{\mu}_0 = \psi(\mathbf{k},\mathbf{n}) \begin{pmatrix} c_1(\mathbf{n}) & c_2(\mathbf{n}) \\ c_2^*(\mathbf{n}) & -c_1(\mathbf{n}) \end{pmatrix}, \tag{13}$$

where $\psi(\mathbf{k},\mathbf{n})$ is some real scalar function of $\mathbf{k}$ and $\mathbf{n}$, while $c_1(\mathbf{n})$ and $c_2(\mathbf{n})$ are some real and complex functions of $\mathbf{n}$, respectively. In the basis in which the matrix $\hat{\mu}_0$ does have the form of Eq. (13), and hence in which the local g-factor approach is valid, the insertion of formula (12) into Eq. (8) leads to the expression

$$g = \pm \frac{2m}{\pi m^*} \oint_\Gamma \frac{d\kappa}{v_\perp} \left(\sqrt{(\mu_{0,11})^2 + |\mu_{0,12}|^2} \right), \tag{14}$$

while the local g factor can be defined as follows,

$$g(\mathbf{k}) = \pm \frac{4m}{\hbar} \sqrt{[\mu_{0,11}(\mathbf{k})]^2 + |\mu_{0,12}(\mathbf{k})|^2}. \tag{15}$$

Note that Eqs. (15) and (14) agree with formulas (6) and (7). Indeed, at constant τ, the matrix $\hat{U}$ transforming $\hat{\mu}_0(\mathbf{k})$ to the diagonal form is also constant; the second term in Eq. (11) vanishes, and the diagonal elements of the transformed matrix $\hat{\mu}_0(\mathbf{k})$ are equal to $\pm[\mu_{0,11}^2(\mathbf{k}) + |\mu_{0,12}(\mathbf{k})|^2]^{1/2}$.

In general case, the matrix μ_0 does not seem to reduce to form (13), and therefore the local g-factor approach is not true. However, when the spin-orbit interaction is absent, the matrix $\hat{\mu}_0$ has just this form. Moreover, as was shown in our previous paper,[8] the local g-factor approach is approximately valid if the strength of the spin-orbit interaction in the crystal is sufficiently weak. To describe the strength of this interaction, we introduced the parameter

$$\nu \equiv \frac{\Delta}{E_0}, \tag{16}$$

where Δ is a characteristic spin-orbit energy in the crystal, while $E_0 \sim mv^2$ is a typical energy scale of an electron-band structure in it (v describes a characteristic value of interband matrix elements of velocity, and E_0 is of the order of the atomic energies, $E_0 \sim 0.1-1\,\mathrm{Ry}$). When the spin-orbit interaction in the crystal is strong, i.e., $\nu \sim 1$, one may expect that only formulas (8), (9), and (10) can give the correct results for the g factor, while the local g-factor approach is not valid at all. Below we investigate this issue in more detail for various types of the electron-band structures and show that this is not always the case.

1. "One-band" case

Consider the case when the Fermi energy ε_F lies near a minimum or a maximum of $\varepsilon_0(\mathbf{k})$ occurring at a point $\mathbf{k}_{ex}$ of the Brillouin zone,

$$\min_{n\neq 0}\left|\frac{\varepsilon_F-\varepsilon_0(\mathbf{k}_{ex})}{\varepsilon_n(\mathbf{k}_{ex})-\varepsilon_0(\mathbf{k}_{ex})}\right|\ll 1.$$

In this situation the orbit Γ is small and is located near this point. The quantities $\mu_{0,\rho\rho'}(\mathbf{k})$ are approximately constant in the orbit, $\mu_{0,\rho\rho'}(\mathbf{k})\approx\mu_{0,\rho\rho'}(\mathbf{k}_{ex})$, and the matrix $\hat{\mu}_0$ has the form of Eq. (13). Thus, in this case, the local *g*-factor approach leads to the exact results for the *g* factor at *arbitrary* strength of spin-orbit interaction. Using Eq. (14), we find that the *g*-factor of the orbit coincides with the local *g* factor and is given by the formula

$$g=\pm\frac{4m}{\hbar}\sqrt{(\mu_{0,11}(\mathbf{k}_{\rm ex}))^2+|\mu_{0,12}(\mathbf{k}_{\rm ex})|^2}. \tag{17}$$

Note that expression (17) fully agrees with formula (26) of Ref. 34 if one takes into account that $\mathbf{v}_0(\mathbf{k}_{\rm ex})=0$.

2. Two-band case

A two-band model can be applied to real situations if in some region of the Brillouin zone, the energy gap between the band under consideration $\varepsilon_0(\mathbf{k})$ and some other band $\varepsilon_a(\mathbf{k})$ as well as the energy differences between these bands and the Fermi energy ε_F are all relatively small as compared to other energy intervals: $|\varepsilon_0(\mathbf{k})-\varepsilon_a(\mathbf{k})|$, $|\varepsilon_F-\varepsilon_0(\mathbf{k})|\ll|\varepsilon_n(\mathbf{k})-\varepsilon_0(\mathbf{k})|$, for $n\neq 0,a$. Then, in this region of the Brillouin zone, one may take into account only the bands 0 and *a* and neglect all other bands. In other words, in this region, we can use the following **kp** Hamiltonian

$$(\hat{H}_{LK})_{l\rho,l'\rho'}=\varepsilon_l(0)\,\delta_{ll'}\delta_{\rho\rho'}+\hbar\mathbf{v}_{l\rho,l'\rho'}(0)\mathbf{k}, \tag{18}$$

where $l, l'=0, a$; $\rho, \rho'=1, 2$; the vector $\mathbf{k}$ is measured from a point taken inside the region [it is convenient to place the point $\mathbf{k}=0$ at the point of an extremum of $\varepsilon_0(\mathbf{k})$]. The basis functions of this Hamiltonian are the well-known functions of Luttinger-Kohn,[35] $\chi_{\mathbf{k},l\rho}=\exp(i\mathbf{kr})\psi_{\mathbf{0},l\rho}$, which coincide with the Bloch functions $\psi_{\mathbf{k},l\rho}$ at the point $\mathbf{k}=0$. Note that in Eq. (18), a diagonal term[35] proportional to k^2 was omitted since its effect on the spectrum is comparable with an effect of the bands disregarded here. The symmetry relative to spatial and time inversion leads[34] to the following relationships between $\mathbf{v}_{l\rho,l'\rho'}(0)$:

$$\begin{aligned}
&\mathbf{v}_{01,01}(0)=\mathbf{v}_{02,02}(0)\equiv\mathbf{v}_0(0),\\
&\mathbf{v}_{a1,a1}(0)=\mathbf{v}_{a2,a2}(0)\equiv\mathbf{v}_a(0),\\
&\mathbf{v}_{02,a2}(0)=\mathbf{v}^*_{01,a1}(0),\\
&\mathbf{v}_{02,a1}(0)=-\mathbf{v}^*_{01,a2}(0).
\end{aligned} \tag{19}$$

The electron dispersion relations $\varepsilon_l(\mathbf{k})$ for the bands 0 and *a* are obtained by diagonalization of Eq. (18):

$$[\hat{S}^+\hat{H}_{LK}\hat{S}]_{l\rho,l'\rho'}=\varepsilon_l(\mathbf{k})\,\delta_{ll'}\delta_{\rho\rho'}, \tag{20}$$

where $\hat{S}$ is an unitary transformation. It is worth noting that the two-band model of the energy spectrum (18) is more general than that of Ref. 34, since we do not assume here that the velocities $\mathbf{v}_0=(1/\hbar)(\partial\varepsilon_0/\partial\mathbf{k})$ and $\mathbf{v}_a=(1/\hbar)(\partial\varepsilon_a/\partial\mathbf{k})$ vanish at *the same* point of the Brillouin zone. In other words, we admit possibility that the bands 0 and *a* reach an extremum at different points of the Brillouin zone.

In our previous paper (Appendix of Ref. 8) we showed how to obtain the orbital part of the matrix $\hat{\mu}_0$ using the Hamiltonian in the Luttinger-Kohn representation $\hat{H}_{LK}$ and the matrix $\hat{S}$ which transforms it to the diagonal form (i.e., to the Bloch representation). This formula can be rewritten in the form:

$$\mu^{or}_{0,\rho\rho'}=\frac{i}{2\hbar}\sum_{\alpha,\beta,\gamma=1,2,3}e_{\alpha\beta\gamma}n_\gamma \times\left\{\hat{S}^+\left(\frac{\partial\varepsilon_0}{\partial k_\alpha}\mathbb{1}+\frac{\partial\hat{H}_{LK}}{\partial k_\alpha}\right)\frac{\partial\hat{S}}{\partial k_\beta}\right\}_{0\rho,0\rho'}, \tag{21}$$

where $e_{\alpha\beta\gamma}$ is the completely antisymmetric tensor which has values ± 1. The spin contribution to $\hat{\mu}_0$ may be neglected here, since this contribution is comparable with that of the disregarded bands. Using Eqs. (18) and (21), we find that the matrix $\hat{\mu}_0$ has the form of Eq. (13) with

$$\psi(\mathbf{k})=\frac{\hbar[\varepsilon_F+0.5E_g-\hbar\mathbf{v}_a(0)\mathbf{k}]^{-1}}{2\varepsilon_F-\hbar[\mathbf{v}_0(0)-\mathbf{v}_a(0)]\mathbf{k}} \tag{22}$$

and

$$c_j=(\mathbf{nw}_j)\left(\varepsilon_F+\frac{E_g}{2}\right)-\hbar k_H[\mathbf{n}\times\mathbf{w}_j]\cdot[\mathbf{n}\times\mathbf{v}_a(0)], \tag{23}$$

where $j=1, 2$; the Fermi energy ε_F is measured from the middle of the gap $E_g=\varepsilon_0(0)-\varepsilon_a(0)$ at the point $\mathbf{k}=0$, and we have used the notations: $k_H=(\mathbf{nk})$,

$$2\mathbf{w}_1=i[\mathbf{v}_{01,a1}(0)\times\mathbf{v}_{02,a2}(0)]-i[\mathbf{v}_{01,a2}(0)\times\mathbf{v}_{02,a1}(0)],$$

$$\mathbf{w}_2=i[\mathbf{v}_{01,a2}(0)\times\mathbf{v}_{01,a1}(0)].$$

Thus, within the two-band approximation, the local *g*-factor approach leads to the exact results for the *g*-factor at *arbitrary* strength of spin-orbit interaction. Using Eq. (14), we find the *g* factor of the orbit,

$$g=\pm\frac{2m}{\pi m^*}\sqrt{c_1^2+|c_2|^2}\oint_\Gamma\frac{d\kappa}{v_\perp}\psi(\mathbf{k}), \tag{24}$$

while the local *g* factor can be defined by the expression $g(\mathbf{k})=\pm(4m/\hbar)\sqrt{c_1^2+|c_2|^2}\psi(\mathbf{k})$.

In the special case $\mathbf{v}_0(0)=\mathbf{v}_a(0)=0$ and $\varepsilon_F\to\varepsilon_0(0)$, the *g* factor of the orbit was calculated by Cohen and Blount,[34] and it was shown that $\delta\equiv(gm^*)/(4m)=\pm 1/2$, i.e., the splitting of the electron energy levels in the magnetic field described by the *g* factor *exactly* coincides with their orbital

TABLE I. Band parameters of bismuth. (Ref. 39). The Fermi energy of electrons in Bi is $\varepsilon_F = 35$ meV.

q_1(a.u.)	$\lvert q_2\rvert$(a.u.)	q_3(a.u.)	α_0(a.u.)	α_a(a.u.)	E_g (meV)
0.457	0.03	0.344	0.615	1.1	10

splitting. We now can extend this result to the general case when ε_F is not close to the band edge $\varepsilon_0(0)$ and the velocities $\mathbf{v}_0$, $\mathbf{v}_a$ do not vanish at the same point of the Brillouin zone. Indeed, inserting Eqs. (22) and (23) into formula (24), we find by a direct calculation that $\delta = 1/2$. Note also that this result agrees with the exact calculation of the electron energy spectrum in the magnetic field.[36]

3. Three or more bands

In our previous paper[8] we calculated the g factor for a three-band model of the electron energy spectrum. This model is commonly used to describe a part of the Fermi surface of zinc, the so-called needles located near the points K of the Brillouin zone. The g-factor of zinc is large due to very small gaps in the spectrum at the point K (the gaps are comparable with the spin-orbit splitting Δ). However, in zinc the parameter Δ is small as compared to the characteristic energy E_0 (i.e., $\nu \ll 1$), and so the local g-factor approach is a good approximation. If one formally increases the strength of the spin-orbit interaction in this three-band model so that the Δ becomes comparable to E_0, formulas (25) and (26) of Ref. 8 show that the matrix $\hat{\mu}_0$ is not reduced to the form of Eq. (13). Thus, this example demonstrates that in the case of a sufficiently strong spin-orbit coupling, the local g-factor approach generally fails when one deals with three (or more) band models of the electron spectrum.

III. BISMUTH

To consider an example of the spectrum with more than two bands and with the strong spin-orbit interaction, we now analyze the electron g factor of bismuth. The electron Fermi surface of Bi consists of three ''ellipsoids'' located near the symmetry points L of the Brillouin zone.[1,31] The symmetry of this point is C_{2h}. It is a common practice to take the x axis along the twofold axis C_2, to place the y-z plane on the reflection plane σ_h containing the trigonal axis C_3 and the bisector axis C_1, and to choose the y axis in the direction of the longest principal axis of the ellipsoid (this axis is approximately ten times greater than the other two and is tilted at the angle about 6 deg from the C_1 axis). 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 extended two-band model, Appendix B, is commonly used. In the case of bismuth, the quadratic terms are taken into account only for this direction. Then, we arrive at the Hamiltonian of McClure[37,38]

$$\hat{\tilde{H}}(\mathbf{k}) = \begin{pmatrix} E_0(\mathbf{k})\mathbb{1}_{2\times 2} & \hat{T}(\mathbf{k}) \\ \hat{T}^{+}(\mathbf{k}) & E_a(\mathbf{k})\mathbb{1}_{2\times 2} \end{pmatrix}, \tag{25}$$

where the point $\mathbf{k}=0$ is placed at the L point;

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

$$\hat{T}(\mathbf{k}) = \begin{pmatrix} t & u \\ -u^* & t^* \end{pmatrix};$$

$$t = q_1 k_x; \quad u = q_2 k_y + q_3 k_z;$$

$E_g = \varepsilon_0(0) - \varepsilon_a(0)$, α_0, α_a, q_1, and q_3 are real parameters of the model, while q_2 is an imaginary constant, $\mathrm{Re}(q_2)=0$. Values of all these parameters are well known,[39,40] see Table I. The parameters q_1, q_2, q_3 denotes the nonzero components of $\hbar \mathbf{v}_{0\rho,a\rho'}(0)$. Note that the value of q_2 is relatively small, and just for this reason the Fermi surface is elongated in the k_y direction, and $\lvert q_2\rvert k_y \sim \lvert \alpha_{0,a} k_y^2\rvert$ at the Fermi level. The equation for the band energies $\varepsilon_0(\mathbf{k})$ and $\varepsilon_a(\mathbf{k})$ follows from Eqs. (25) and (B5):

$$\left[\varepsilon - \frac{(\alpha_0 - \alpha_a)k_y^2}{4}\right]^2 = \left[\frac{E_g}{2} + \frac{(\alpha_0 + \alpha_a)k_y^2}{4}\right]^2 + q_1^2 k_x^2 + |q_2|^2 k_y^2 + q_3^2 k_z^2, \tag{26}$$

where the energy ε is measured from the middle of the energy gap E_g at the point L.

The constant matrices $\hat{R}_\gamma$, Appendix B, considerably simplify if one takes into account the symmetry of the point L:

$$\hat{R} \equiv \sum_{\gamma=1,2,3} \hat{R}_\gamma n_\gamma = \begin{pmatrix} \hat{\rho}_0 & 0 \\ 0 & \hat{\rho}_a \end{pmatrix}, \tag{27}$$

where

$$\hat{\rho}_{0,a} = \begin{pmatrix} \tilde{\rho}_{0,a} & \tilde{\nu}_{0,a} \\ \tilde{\nu}^*_{0,a} & -\tilde{\rho}_{0,a} \end{pmatrix}$$

are the 2×2 matrices with

$$\tilde{\rho}_{0,a} = \rho_{0,a} n_x, \quad \tilde{\nu}_{0,a} = \nu^y_{0,a} n_y + \nu^z_{0,a} n_z.$$

The two real constants ρ_0, ρ_a, and four complex parameters ν_0^y, ν_a^y, ν_0^z, ν_a^z represent both the effect of bands different from 0 and a on the matrix $\hat{\mu}_0$ and the pure spin part $\hat{\mu}_0^s$. Substituting Eq. (27) into formula (B8), we obtain the matrix elements of $\hat{\mu}_0$ for central cross sections of the Fermi surface

$$\mu_{0,11} = A[iBq_2q_3n_x + \tilde{\rho}_0(E_a - \varepsilon_F)^2 + \tilde{\rho}_a(t^2 - |u|^2) + t(\tilde{\nu}_a u^* + \tilde{\nu}_a^* u)]$$

$$\mu_{0,12}=A[iBq_1(q_3n_y-q_2n_z)-2\tilde{\rho}_a tu + \tilde{\nu}_0(E_a-\varepsilon_F)^2+\tilde{\nu}_a t^2-\tilde{\nu}_a^* u^2], \quad (28)$$

where

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

$$B=(E_a+E_g+\varepsilon_F)/\hbar. \quad (29)$$

Since $\rho_{0,a}$ and $\nu_{0,a}^{y,z}$ are all of the order of $\hbar/m$, the terms in Eq. (28) proportional to these parameters are relatively small as compared to the main terms which contain products of q_i and result from $\hat{\mu}_0^{(2)}$, Eq. (B9). If the magnetic field is directed along the y axis, the small terms with $\tilde{\rho}_{0,a}$ and $\tilde{\nu}_{0,a}$ can be omitted. Then, we go over to the case of the two-band model, and the matrix $\hat{\mu}_0$ takes the form of Eq. (13),

$$\hat{\mu}=|\mu_{0,12}|\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}.$$

Thus, one arrives at

$$\delta\equiv\frac{gm^*}{4m}=\pm\frac{1}{2}.$$

If $n_y\ll 1$, i.e., if the magnetic-field direction is almost normal to the y axis, the role of the terms with $\tilde{\rho}_{0,a}$ and $\tilde{\nu}_{0,a}$ increases due to the small value of q_2. In this case, the matrix $\hat{\mu}_0$ cannot be reduced to the form of Eq. (13), and to obtain the electron g factor, one must use Eqs. (8), (9), and (10).

The angular dependence of the electron g factor of bismuth in the y-z plane was very accurately measured in Ref. 31, see Fig. 1. In Fig. 1 we also show the electron g factor calculated using Eqs. (8), (9), (10), (28), and the data of Tables I, and II. If one neglects the terms with $\nu_{0,a}^{y,z}$, the calculated g factor only qualitatively agrees with the experimental data, but it is impossible to obtain their quantitative agreement. In particular, these terms determine the asymmetry of the plot relative to the direction of the z axis. The values of the parameters $\nu_{0,a}^{y,z}$ have been chosen so that to provide the best agreement of the calculated g factor with the experimental data. It should be noted that this choice is not unique, and the Table II gives only one possible set of the values. In this context, we point out that the experimental investigation of angular dependences of the g factor in the x-z and the x-y planes would enable one to determine the parameters unambiguously.

The results of Fig. 1 are in agreement with the considerations presented above. If the magnetic-field direction **n** is close to the y axis, the combination $\delta=(gm^*/4m)$ approaches the value 1/2. But when **n** is almost perpendicular to the y axis, the magnitude of the δ significantly differs from this value characteristic for the two-band model of the electron energy spectrum.

We have compared the exact g factor calculated using Eqs. (8), (9), and (10) with that calculated on the basis of formula (14), see Fig. 2. When the magnetic-field direction **n** is not close to the x-z plane, the results of the two approaches practically coincide. But when **n** lies near the x-z plane [i.e., when the two-band model fails and formula (14) is not valid], the comparison clearly shows the error which occurs if one continues to use Eq. (14). Hence, the formal use of Eq. (14) in this region of the magnetic-field directions can lead to a noticeable error in the g factor. It should be emphasized that this conclusion is independent of the set of the values in Table II.

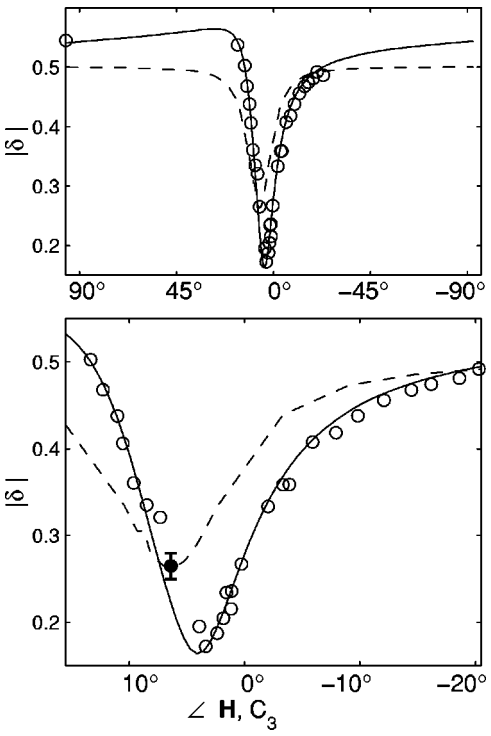

FIG. 1. The quantity $|\delta|=|gm^*/4m|$ for electron orbits in bismuth as functions of angle between the direction of the magnetic field **H** and the trigonal axis C_3 of the crystal; **H** lies in the y-z plane. The solid line is plotted using Eqs. (8), (9), (10), (28) and the data of Tables I and II, while ○ marks the experimental data (Ref. 31). The lower panel shows the results near the trigonal axis in an enlarged scale. The filled circle corresponds to z direction, and only for this point the error bars are shown. The dashed line represents the exact g factor calculated at all $\nu_{0,a}^{y,z}=0$.

IV. CONCLUSIONS

In the semiclassical approximation the electron g factor in metals can be calculated using formulas (8), (9), and (10). Within this approach, Eq. (9) with boundary condition (10) describes the dynamics of the electron spin when the electron moves over the semiclassical orbit in the crystal. On the other hand, in many papers, the so-called local g-factor ap-

TABLE II. A possible set of the parameters $\rho_{0,a}$, $\nu_{0,a}^y$, $\nu_{0,a}^z$ for bismuth (atomic units). ρ_0 and ρ_a were chosen using the known data for the electron g factor in the x direction (Ref. 31).

ν_0^y	ν_0^z	ν_a^y	ν_a^z	ρ_0	ρ_a
2+5i	-1+2i	2+5i	-1+2i	1.7	-7.4

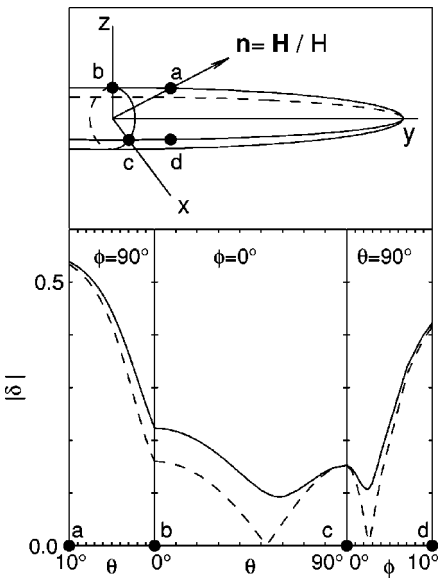

FIG. 2. The quantity $|\delta|=|gm^*/4m|$ calculated using Eqs. (8), (9), (10) (the solid lines), and using Eq. (14) (the dashed lines) for bismuth when the magnetic-field direction $\mathbf{n}=\mathbf{H}/H=(\sin\theta\cos\varphi,\sin\theta\sin\varphi,\cos\theta)$ lies in the y-z, z-x, and x-y planes. The upper panel shows a half of the electron ellipsoid of bismuth and positions of the points a-d marked in the lower panel. The calculations were carried out using formulas (28) and the data of Tables I and II; $|\delta|$ has been reduced to the interval 0–1/2.

proach was applied to calculate the electron g factors of a number of metals. This simple approach is applicable only if the dynamics of the electron spin is negligible. In this case one can use formula (14) to calculate the g factor of the electron orbits. We compare these two approaches and find out when they lead to the same g factor and when one should expect a difference in the results.

The local g-factor approach is a good approximation in crystals with a weak spin-orbit coupling. Besides this, there are two situations when this approach leads to the exact results at a strong spin-orbit interaction. In the first case, the Fermi level lies near an edge of the band under consideration. In the second situation, the electron spectrum that specifies the semiclassical orbit can be well described in the framework of the two-band model. In all other cases, one may expect a difference between the exact results and those obtained by the local g-factor approach.

As an example, we consider the g factor of bismuth. If the magnetic field has a direction near the plane containing the trigonal and the binary axes of bismuth, the g factor of the electron orbits cannot be described in the framework of the two-band model, and the effect of other bands on the g-factor (and the spin contribution to it) should be taken into account. In this case the two approaches lead to different results for the g factor.

APPENDIX A: BLOCH BASIS TRANSFORMATIONS AND g FACTOR INVARIANCE

In the case of the crystals with the inversion symmetry, the most general unitary transformation of the spinor space has the form

$$\hat{U}(\mathbf{k})=\begin{pmatrix} c\exp[i\alpha(\mathbf{k})] & -s\exp[i\beta(\mathbf{k})] \\ s\exp[-i\beta(\mathbf{k})] & c\exp[-i\alpha(\mathbf{k})]\end{pmatrix}, \tag{A1}$$

where $c=\cos[\phi(\mathbf{k})]$, $s=\sin[\phi(\mathbf{k})]$, and α, β, ϕ are some real functions of $\mathbf{k}$. This transformation can be decomposed as follows,

$$\hat{U}(\mathbf{k})=\hat{P}\left(\frac{\alpha+\beta}{2}\right)\hat{R}(\phi)\hat{P}\left(\frac{\alpha-\beta}{2}\right), \tag{A2}$$

where $\hat{P}(\eta)$ is the phase transformation

$$\hat{P}(\eta(\mathbf{k}))=\begin{pmatrix}\exp[i\eta(\mathbf{k})] & 0 \\ 0 & \exp[-i\eta(\mathbf{k})]\end{pmatrix}, \tag{A3}$$

and $\hat{R}(\phi)$ is the rotation in the spinor space

$$\hat{R}(\phi(\mathbf{k}))=\begin{pmatrix}\cos\phi(\mathbf{k}) & \sin\phi(\mathbf{k}) \\ -\sin\phi(\mathbf{k}) & \cos\phi(\mathbf{k})\end{pmatrix}. \tag{A4}$$

The phase transformation $\hat{P}(\eta(\mathbf{k}))$ does not change the form of Eqs. (8) and (7).[8] Consider now rotation transformation (A4). It changes the matrix $\hat{\mu}_0(\mathbf{k})$ as follows:

$$\hat{\mu}_0'=\hat{R}^+(\phi)\hat{\mu}_0\hat{R}(\phi)+i\left(\mathbf{n}\left[\mathbf{v}_0\times\hat{R}^+(\phi)\left(\frac{\partial\hat{R}(\phi)}{\partial\mathbf{k}}\right)\right]\right), \tag{A5}$$

and the solution of transformed equation (9) (written with the use of the new matrix elements $\mu'_{0,\rho\rho'}$) has the form

$$\tau'(\mathbf{k})=\frac{\sin\phi(\mathbf{k})+\cos\phi(\mathbf{k})\cdot\tau(\mathbf{k})}{\cos\phi(\mathbf{k})-\sin\phi(\mathbf{k})\cdot\tau(\mathbf{k})}. \tag{A6}$$

Substituting τ' and $\mu'_{0,\rho\rho'}$ into Eq. (8), it can be verified that the change of the exact g factor is described by

$$\frac{m^*}{4m}(g'-g)=\frac{1}{2\pi}\oint_\Gamma d\kappa\frac{d\arg[\cos\phi(\mathbf{k})-\sin\phi(\mathbf{k})\tau(\mathbf{k})]}{d\kappa}$$
$$=n', \tag{A7}$$

where n' is some integer. Since in the semiclassical approach, the change of $\delta\equiv(gm^*)/(4m)$ by arbitrary integer does not affect energy spectrum (1), we can state that the exact expression (8) is really invariant under transformations (A4) [and hence (A1)]. In contrast to this, the rotation in the spinor space (A4) essentially changes expression (7),

$$g'=-\frac{2m}{\pi m^*}\oint_\Gamma\frac{d\kappa}{v_\perp}[\cos(2\phi)\mu_{0,11}-\sin(2\phi)\mathrm{Re}(\mu_{0,12})]. \tag{A8}$$

APPENDIX B: THE EXTENDED TWO-BAND MODEL

There exist situations when the two-band model is not sufficient to describe the electron energy spectrum $\varepsilon_0(\mathbf{k})$ and the matrix $\hat{\mu}_0(\mathbf{k})$ with an appropriate precision even in the case of the two close bands. We now show how to obtain ε_0 and $\hat{\mu}_0$ for the extended two-band model, in which the effect

of other bands on these quantities is taken into account to the first order.

The electron energy spectrum of the extended two-band model can be derived from the Luttinger-Kohn Hamiltonian[35]

$$(\hat{H}_{LK})_{n\rho,n'\rho'}=\left(\varepsilon_n(0)+\frac{\hbar^2\mathbf{k}^2}{2m}\right)\delta_{nn'}\delta_{\rho\rho'}+\hbar\mathbf{v}_{n\rho,n'\rho'}(0)\mathbf{k}, \tag{B1}$$

which includes *all* bands. We carry out the diagonalization of infinite matrix (B1) by some unitary transformation $\hat{S}$ in the two steps: At the first step the matrix elements $(\hat{H}_{LK})_{l\rho,n\rho'}$ between the bands under consideration, $l=0$, a, and the other bands, $n\neq 0$, a, are reduced to zero by an unitary transformation $\hat{S}_1$. At this step we arrive at the following transformed Hamiltonian:

$$\hat{S}_1^+\hat{H}_{LK}\hat{S}_1=\begin{pmatrix}\hat{\tilde{H}}(\mathbf{k}) & 0\\ 0 & \hat{\tilde{H}}_R(\mathbf{k})\end{pmatrix}. \tag{B2}$$

The matrix $\hat{S}_1$ has the form of a series in components of $\mathbf{k}$. Thus, we find that the leading correction to $(\hat{H}_{LK})_{l\rho,l'\rho'}$ is a quadratic form in these components:

$$(\hat{\tilde{H}}-\hat{H}_{LK})_{l\rho,l'\rho'}=\frac{\hbar^2}{2}{\sum_{n,\rho''}}'\,[\mathbf{v}_{l\rho,n\rho''}(0)\mathbf{k}][\mathbf{v}_{n\rho'',l'\rho'}(0)\mathbf{k}]T^n_{ll'}, \tag{B3}$$

where

$$T^n_{ll'}=\frac{1}{\varepsilon_l(\mathbf{0})-\varepsilon_n(\mathbf{0})}+\frac{1}{\varepsilon_{l'}(\mathbf{0})-\varepsilon_n(\mathbf{0})};$$

$l,l'=0,a$, and Σ'_n denotes that the summation excludes $n=0$, a. The lower right block in matrix (B2) describes the bands different from 0 and a and is not considered any more. The second step of the diagonalization is to find a four-dimensional unitary matrix $\hat{S}_2(\mathbf{k})$ that transforms $\hat{\tilde{H}}$ to the diagonal form

$$[\hat{S}_2^+\hat{\tilde{H}}\hat{S}_2]_{l\rho,l'\rho'}=\varepsilon_l(\mathbf{k})\,\delta_{ll'}\delta_{\rho\rho'}. \tag{B4}$$

The matrix $\hat{S}_2(\mathbf{k})$ depends only on the matrix elements of the Hamiltonian $\hat{\tilde{H}}$. The band energies $\varepsilon_0(\mathbf{k})$ and $\varepsilon_a(\mathbf{k})$ are found from the equation

$$\det[\hat{\tilde{H}}-\varepsilon_l(\mathbf{k})]=0. \tag{B5}$$

The matrix elements of $\hat{\mu}_0$ can be obtained from Hamiltonian (B1) using the formulas of the Appendix of Ref. 8. The orbital part of $\hat{\mu}_0$ is given by formula (21) of the present paper, while its spin part $\hat{\mu}_0^s$ has the form

$$\mu^s_{0,\rho\rho'}=\sum_{\gamma=1,2.3}n_\gamma(\hat{S}^+\hat{\Sigma}_\gamma\hat{S})_{0\rho,0\rho'}, \tag{B6}$$

where

$$[\hat{\Sigma}_\gamma]_{n\rho,n'\rho'}=-\frac{\hbar}{2m}\langle\chi_{\mathbf{k},n\rho}|\sigma_\gamma|\chi_{\mathbf{k},n'\rho'}\rangle. \tag{B7}$$

The unitary matrix $\hat{S}$ in these formulas must be taken in the same approximation as in the determination of $\hat{\tilde{H}}$.

The two step procedure enables one to represent matrix elements of $\hat{\mu}_0$ as the sum of the two terms

$$[\hat{\mu}]_{0,\rho\rho'}=\sum_{\gamma=1,2,3}n_\gamma[\hat{S}_2^+\hat{R}_\gamma\hat{S}_2n_\gamma]_{0\rho,0\rho'}+[\hat{\mu}^{(2)}]_{0,\rho\rho'}, \tag{B8}$$

where the second term $\hat{\mu}_0^{(2)}$ depends only on the matrix elements of the Hamiltonian $\hat{\tilde{H}}$ [compare with Eq. (21)]:

$$[\hat{\mu}^{(2)}]_{0,\rho\rho'}=\frac{i}{2\hbar}\cdot\sum_{\alpha,\beta,\gamma=1,2,3}e_{\alpha\beta\gamma}n_\gamma \times\left\{\hat{S}_2^+\left(\frac{\partial\varepsilon_0}{\partial k_\alpha}\mathbb{1}+\frac{\partial\hat{\tilde{H}}}{\partial k_\alpha}\right)\frac{\partial\hat{S}_2}{\partial k_\beta}\right\}_{0\rho,0\rho'}, \tag{B9}$$

while the four-dimensional matrices $\hat{R}_\gamma(\mathbf{k})$ are determined by the bands different from 0, a, and by the contribution (B7) associated with the spin:

$$[\hat{R}_\gamma]_{l\rho,l'\rho'}=\frac{i}{2}\sum_{\alpha,\beta=1,2,3}e_{\alpha\beta\gamma}\left\{\hat{\tilde{\Omega}}_\beta\frac{\partial\hat{\tilde{H}}}{\hbar\,\partial k_\alpha}+\hat{\tilde{v}}_\alpha\hat{\tilde{\Omega}}_\beta\right\}_{l\rho,l'\rho'} +[\hat{S}_1^+\hat{\Sigma}_\gamma\hat{S}_1]_{l\rho,l'\rho'}. \tag{B10}$$

Here

$$\hat{\tilde{v}}_\alpha=\hat{S}_1^+\hat{v}_\alpha\hat{S}_1,\hat{\tilde{\Omega}}_\beta=i\hat{S}_1^+(\partial\hat{S}_1/\partial k_\beta) \tag{B11}$$

and the vector of the matrices $\hat{v}_\alpha$ is defined by the relationships $(\hat{v}_\alpha)_{n\rho,n'\rho'}=v^\alpha_{n\rho,n'\rho'}$. The matrices $\hat{R}_\gamma$ are series in $\mathbf{k}$, and in the approximation used, only the first terms of these series must be taken into account. Therefore, these matrices reduce to the constant matrices:

$$(\hat{R}_\gamma)_{l\rho,l'\rho'}=\frac{i\hbar}{2}{\sum_{n,\rho''}}'\,[\mathbf{v}_{l\rho,n\rho''}(0)\times\mathbf{v}_{n\rho'',l'\rho'}(0)]T^n_{ll'} +(\hat{\Sigma}_\gamma)_{l\rho,l'\rho'}, \tag{B12}$$

which are determined by values of $\hat{R}_\gamma$ at the point $\mathbf{k}=0$. When the point $\mathbf{k}=0$ is a symmetry point of the Brillouin zone, the form of the matrices $\hat{R}_\gamma$ is considerably simplified by the use of the selection rules for the matrix elements of angular momentum.

[1] D. Shoenberg, *Magnetic Oscillations in Metals* (Cambridge University Press, Cambridge, England, 1984).
[2] See, e. g., J.M. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, Cambridge, England, 1972); E.M. Lifshitz and L.P. Pitaevskii, *Statistical Physics* (Pergamon Press, Oxford, 1986), Pt. 2.
[3] L. Onsager, Philos. Mag. **43**, 1006 (1952).
[4] I.M. Lifshits and A.M. Kosevich, Zh. Éksp. Teor. Fiz., **29**, 730 (1955) [Sov. Phys. JETP **2**, 636 (1956)].
[5] G.P. Mikitik and Yu.V. Sharlai, Zh. Éksp. Teor. Fiz, **114**, 1357 (1998) [Sov. Phys. JETP **87**, 747 (1998)].
[6] G.P. Mikitik and Yu.V. Sharlai, Phys. Rev. Lett. **82**, 2147 (1999).
[7] L.M. Roth, Phys. Rev. **145**, 434 (1966).
[8] G.P. Mikitik and Yu.V. Sharlai, Phys. Rev. B **65**, 184426 (2002).
[9] A.W. Overhauser and A.M. De Graaf, Phys. Rev. Lett. **22**, 127 (1969).
[10] A.M. De Graaf and A.W. Overhauser, Phys. Rev. B **2**, 1437 (1970).
[11] R.A. Moore and C.F. Liu, Phys. Rev. B **8**, 599 (1973).
[12] R.A. Moore, J. Phys. F: Met. Phys. **5**, 2300 (1975).
[13] M. Singh, J. Callaway, and C.S. Wang, Phys. Rev. B **14**, 1214 (1978).
[14] T.S. Rahman, J.C. Parlebas, and D.L. Mills, J. Phys. F: Met. Phys. **8**, 2511 (1978).
[15] F. Beuneu, J. Phys. F: Met. Phys. **10**, 2875 (1980).
[16] T. Jarlborg and A.J. Freeman, Phys. Rev. B **23**, 3577 (1981).
[17] A.H. MacDonald, J.M. Daams, S.H. Vosko, and D.D. Koelling, Phys. Rev. B **25**, 713 (1982).
[18] H. Ohlsen, P. Gustafsson, L. Nordborg, and S.P. Hornfeldt, Phys. Rev. B **29**, 3022 (1984).
[19] C. Shober, G. Kurz, H. Wohn, V.V. Nemoshkalenko, and V.N. Antonov, Phys. Status Solidi B **136**, 233 (1986).
[20] H. Ohlsen, J.L. Calais, Phys. Rev. B **35**, 7914 (1987).
[21] G.E. Grechnev, N.V. Savchenko, I.V. Svechkarev, A.V. Zhalko-Titarenko, M.J.G. Lee, and J.M. Perz, Fiz. Nizk. Temp. **13**, 1219 (1987) [Sov. J. Low Temp. Phys. **13**, 689 (1987)].
[22] N.V. Savchenko and G.E. Grechnev, Fiz. Nizk. Temp. **15**, 656 (1989) [Sov. J. Low Temp. Phys. **15**, 370 (1989)].
[23] G.E. Grechnev, N.V. Savchenko, I.V. Svechkarev, M.J.G. Lee, and J.M. Perz, Phys. Rev. B **39**, 9865 (1989).
[24] O. Eriksson, H. Ohlsén, and J.L. Calais, Phys. Rev. B **40**, 5961 (1989).
[25] A. Hjelm and J.L. Calais, Phys. Rev. Lett. **67**, 2064 (1991).
[26] N.V. Savchenko, Fiz. Nizk. Temp. **17**, 77 (1991) [Sov. J. Low Temp. Phys. **17**, 41 (1991)].
[27] N.V. Savchenko, G.E. Grechnev, and I.V. Svechkarev, Fiz. Nizk. Temp. **17**, 859 (1991) [Sov. J. Low Temp. Phys. **17**, 449 (1991)].
[28] A. Hjelm and J.L. Calais, Phys. Rev. B **48**, 8592 (1993).
[29] V.I. Smelyansky, M.J.G. Lee, and J.M. Perz, J. Phys.: Condens. Matter **5**, 6061 (1993).
[30] A.M. DeGraaf and A.W. Overhauser, Phys. Rev. B **180**, 701 (1969).
[31] V.S. Édelm'man, Usp. Fiz. Nauk **123**, 257 (1977) [Sov. Phys. Usp. **20**, 819 (1977)]; V.S. Édelm'man, Zh. Éksp. Teor. Fiz. **64**, 1734 (1973) [Sov. Phys. JETP **37**, 875 (1973)].
[32] E.I. Blount, Phys. Rev. **126**, 1636 (1962).
[33] L.M. Roth, J. Phys. Chem. Solids **23**, 433 (1962).
[34] M.H. Cohen and E.I. Blount, Philos. Mag. **5**, 115 (1960).
[35] J.M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).
[36] G.P. Mikitik and Yu.V. Sharlai, Fiz. Nizk. Temp. **22**, 762 (1996) [Low Temp. Phys. **22**, 585 (1996)].
[37] J.W. McClure, J. Low Temp. Phys. **25**, 527 (1976).
[38] In the case of bismuth, the subscripts "0" and "a" are frequently denoted by "c" and "v," respectively.
[39] S.Sh. Akhmedov, R. Herrmann, K.N. Kashirin, A. Krapf, V. Kraak, Ya.G. Ponomarev, and M.V. Sudakova, Zh. Éksp. Teor. Fiz. **97**, 663 (1990) [Sov. Phys. JETP **70**, 370 (1990)].
[40] G.P. Mikitik and Yu.V. Sharlai, Fiz. Nizk. Temp. **26**, 54 (2000) [Low Temp. Phys. **26**, 39 (2000)].