g factor of conduction electrons in the de Haas–van Alphen effect

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Although formulas for the semiclassical electron *g* factor in the de Haas–van Alphen effect were first derived by Roth in 1966, they are sufficiently complicated and have not been used in practice so far. In this paper we represent the formulas in a more convenient form which also admits a simple physical interpretation. It follows from these formulas that numerous computations of the *g* factor performed earlier did not take into account the spin dynamics of a semiclassical Bloch electron moving in a magnetic field. This can lead to inaccurate results for the *g* factor if the spin-orbit interaction in the crystal under study is not small. We also point out that the concept of local *g* factors widely used in the computations has a limited field of application and is not generally correct for a strong spin-orbit coupling. Finally, we calculate and analyze the *g* factor for a three-band model of the electron spectrum which was previously used in describing the so-called needles in zinc.

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I. INTRODUCTION

A *g* factor of conduction electrons in a crystal, *g*, specifies the splitting of Landau energy levels caused by an interaction of the electron spin with a magnetic field, $\Delta E = g(e\hbar/2mc)H$. 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). The electron *g* factor in the crystal can considerably differ from its free-electron value, $g=2$, and this difference is due to spin-orbit coupling (here we do not consider the exchange-correlation enhancement of the *g* factor). In metals, the *g* factors are experimentally found from oscillation phenomena (e.g., the de Haas–van Alphen effect) and from electron paramagnetic resonance.[1] In this paper we restrict our consideration to the *g* factors recovered from oscillation effects which are known to occur under the condition $\omega_c t_{sc} > 1$, where ω_c is the cyclotron frequency of the electron and t_{sc} is the electron-scattering time.

In what follows we treat the *g* factor only in the semiclassical limit when there are a lot of the Landau levels under the Fermi surface. Besides this, the magnetic breakdown is assumed not to play any role in the case under study. As well known,[2] under these conditions 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 absence of the magnetic field, $\varepsilon(\mathbf{k}) = \text{const}$, with the plane $k_z = \text{const}$, where z is the direction of the external magnetic field $\mathbf{H}$. In this approach the semiclassical *g* factor appears in the well-known quantization rule[3,4,1] for electron energy ε in a magnetic field,

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

where S is the cross-sectional area of the *closed* orbit Γ, n is a large integer, the cyclotron mass $m^* = (\hbar^2/2\pi)\times(\partial S(\varepsilon,k_z)/\partial\varepsilon)$, the constant γ is always equal to 1/2 when the spin-orbit interaction is taken into account,[5,6] and the *g* factor $g(\varepsilon,k_z)$ depends on a location of the *orbit* Γ in the Brillouin zone. It should be noted that formulas for the *g* factor in terms of electron band parameters were, in fact, derived by Roth,[7] but these formulas are sufficiently complicated and inconvenient to calculate the *g* factor in real situations.

Calculation of the *g* factors were carried out for various metals.[8–29] However, it is necessary to stress that in all these computations Roth's results[7] were not employed, and the approaches commonly used differ from that of Roth mainly in two respects. First, it was common practice to calculate the so-called local *g* factors $g(\mathbf{k})$, introduced in Ref. 30 for *points* $\mathbf{k}$ on the Fermi surface, while the *g* factor for an orbit Γ was obtained by the integration of $g(\mathbf{k})$ over this trajectory Γ. In contrast to this, only the *g* factors of closed *orbits* have a physical meaning in Roth's theory, and a point $\mathbf{k}$ of the Fermi surface can give different contributions to the *g* factors for different orbits passing through this point. Second, while Roth's approach is based on the effective one band Hamiltonian of a Bloch electron in a magnetic field,[31,32] most of the *g*-factor computations used another Hamiltonian which does not take into complete account the influence of the magnetic field on the electron. All these disagreements with the exact theory[7] show that an analysis of the existing approaches to the *g*-factor calculations is required.

In this paper, in Sec. II, we present Roth's results[7] for the *g* factor in the form which admits a simple physical interpretation. In essence, another way of their derivation is outlined here. We also clarify distinctions between the approaches of Roth and of the other authors and point out situations for which the approaches may lead to different results. In Sec. III the *g* factor of electron states forming the so-called needles in zinc is found and analyzed on the basis of the obtained results. The derived expressions generalize the formulas[33] obtained in the vicinity of band edges of Zn and well agree with the experimental data[34] if the appropriate values[35] of the band parameters are used. In the Appendix we give several useful formulas that simplify calculations of the *g* factor for real electron-band structures.

II. FORMULAS FOR g FACTOR

A. Hamiltonian

The quantization rule (1) can be derived using the effective one-band Hamiltonian $\hat{H}_{eff}$ of a Bloch electron in a magnetic field.[31,32] Since electron bands are twofold degenerate in crystals with the inversion symmetry,[2] the Hamiltonian is a 2×2 matrix in spinor space. According to Refs. 31 and 32, this Hamiltonian to first order in the magnetic field H has the form

$$\hat{\mathsf{H}}_{eff}=\varepsilon_0(\hat{\mathbf{k}})\hat{\mathbb{1}}+\frac{e}{c}H\hat{\mu}_0(\hat{\mathbf{k}}), \tag{2}$$

where $\varepsilon_0(\mathbf{k})$ is the electron dispersion relation for the band being investigated (from here on we denote this band by the subscript 0),

$$\hat{\mathbf{k}}=\mathbf{K}-\frac{e}{c\hbar}\mathbf{A}\left(i\frac{\partial}{\partial\mathbf{K}}\right),$$

$\mathbf{A}(\mathbf{r})$ 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 $\mu^{s}_{0,\rho\rho'}$,

$$\mu^{s}_{0,\rho\rho'}(\mathbf{k})=-\frac{\hbar}{2m}\int_{v}u^{*}_{\mathbf{k},0\rho}(\mathbf{r})\sigma_3 u_{\mathbf{k},0\rho'}(\mathbf{r})d\mathbf{k}, \tag{3}$$

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

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

where the spin indexes $\rho,\rho',\rho''=1,2$; σ_3 is the third Pauli matrix; $\mathbf{v}_0=(1/\hbar)(\partial\varepsilon_0/\partial\mathbf{k})$; $\mathbf{v}_{n\rho,m\rho'}$ 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,

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

In what follows we always assume 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.[36] It is also important to emphasize here that the quantities $(e/c)\mu_{0,\rho\rho'}$ do not generally coincide with the matrix elements $M^{z}_{0,\rho\rho'}$ of the z component of the electron magnetic momentum in the $\mathbf{k}$ representation; viz., one has

$$\frac{e}{c}\mu_{0,\rho\rho'}=\frac{e}{2c}[\mathbf{v}_0\times\mathbf{\Omega}_{0\rho,0\rho'}]_z+M^{z}_{0,\rho\rho'}. \tag{6}$$

The difference results from the fact that components of $\hat{\mathbf{k}}$ in $\varepsilon_0(\hat{\mathbf{k}})$ [see Eq. (2)] do not commute.[31,32]

B. Roth's results

As well known,[1] the de Haas–van Alphen effect can be observed when the electron-scattering time t_{sc} exceeds the period of the electron motion in the orbit, $\omega_c t_{sc}>1$. Under this condition a steady state of the electron in the magnetic field is realized, with an energy corresponding to one of the Landau levels. In other words, the electron state looks like a standing wave in the semiclassical orbit. The quantization condition (1) together with the expression for the g factor can be obtained as follows:[5] Using the Hamiltonian (2), one finds the semiclassical wave function of the electron to the second order in the small parameter $1/n$ where n is the ordinal number of the Landau level, and then imposes the constraint that the wave function be single valued; i.e., its phase change over the semiclassical orbit must be equal to $2\pi n$. At given n, two wave functions differing in a direction of the electron spin satisfy this condition. In the representation of the Hamiltonian (2), they have the form $f_+(\mathbf{k})|e(\mathbf{k})\rangle$, $f_-(\mathbf{k})|e_\perp(\mathbf{k})\rangle$, where the unit vectors in the spinor space, $|e\rangle$ and $|e_\perp\rangle$, specify directions of the spin in these two mutually orthogonal states. The scalar functions $f_+(\mathbf{k})$ and $f_-(\mathbf{k})$ are not small only near the semiclassical orbits Γ_+ and Γ_- corresponding to the above-mentioned wave functions (note that the trajectories Γ_+ and Γ_- slightly differ from each other and from Γ defined above[30]). A difference in energies of these two electron states just specifies the g factor.

To describe $|e(\mathbf{k})\rangle$, we shall use the following parametrization:

$$|e\rangle=\frac{1}{\sqrt{(1+|\tau|^2)}}\begin{pmatrix}1\\ \tau\end{pmatrix},$$

where τ is a complex scalar function of $\mathbf{k}$. Then, one has

$$|e_\perp\rangle = \frac{1}{\sqrt{(1+|\tau|^2)}}\begin{pmatrix} \tau^* \\ -1 \end{pmatrix}.$$

Multiplying the Shrödinger equation

$$\hat{H}_{eff} f_+ |e\rangle = \varepsilon_+ f_+ |e\rangle \tag{7}$$

by $\langle e_\perp|$ from the left, we arrive at the equation specifying the function $\tau(\mathbf{k})$ along the semiclassical orbit:

$$i v_\perp \frac{d\tau}{d\kappa} = \mu_{0,12}\tau^2 + 2\mu_{0,11}\tau - \mu^*_{0,12}, \tag{8}$$

where $v_\perp$ is the absolute value of projection of $\mathbf{v}$ on the plane normal to $\mathbf{H}$, and $d\kappa$ is the infinitesimal element of the orbit. In deriving this equation only terms of the leading nonvanishing order in H (i.e., in $1/n$) have been kept, and we have used the formula

$$\langle e_\perp|\varepsilon_0(\hat{\mathbf{k}})|e\rangle = -\frac{e}{\hbar c}\langle e_\perp|\mathbf{v}_0\mathbf{A}\left(i\frac{\partial}{\partial \mathbf{k}}\right)|e\rangle.$$

Taking into account the well-known relation[2] $(d\kappa/v_\perp) = (eH/c)dt$, Eq. (8) can be also considered as an 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). However, in the steady state the direction of the electron spin must periodically return to its initial value. Thus, we arrive at the following boundary condition to Eq. (8):

$$\tau(0) = \tau(\kappa_0), \tag{9}$$

where τ is written as a function of a length along the electron trajectory and κ_0 is the perimeter of the orbit.

Multiplying the Shrödinger equation (7) by $\langle e|$ from the left, neglecting terms of the order of H^2 and higher, and using Eq. (8), we find the equation in the function f_+,

$$\varepsilon_{0\uparrow}(\hat{\mathbf{k}}) f_+ = \varepsilon f_+, \tag{10}$$

which can be considered as the equation for a spinless ''electron'' in the magnetic field with a modified dispersion relation $\varepsilon_{0\uparrow}(\mathbf{k})$. Here $\varepsilon_{0\uparrow}(\mathbf{k})$ has the form

$$\varepsilon_{0\uparrow}(\mathbf{k}) = \varepsilon_0(\mathbf{k}) + \frac{eH}{c}\{\mu_{0,11}(\mathbf{k}) + \Re[\mu_{0,12}(\mathbf{k})\tau(\mathbf{k})]\}. \tag{11}$$

Note that an equation in f_- is similar to Eq. (10), but the appropriate $\varepsilon_{0\downarrow}(\mathbf{k})$ is obtained from formula (11) by changing the sign before (eH/c). Using the well-known quantization rule[3,4] for a spinless particle with the dispersion relation (11), one arrives at

$$S_+(\varepsilon, k_z) = \frac{2\pi|e|H}{\hbar c}\left(n + \frac{1}{2}\right), \tag{12}$$

where S_+ is the cross-sectional area of the orbit Γ_+ defined by the equality $\varepsilon_{0\uparrow}(\mathbf{k}) = \varepsilon$, at a constant k_z. Since H is relatively small, and thus the orbits Γ and Γ_+ are close to each other, one can express S_+ through the area S of the orbit Γ,

$$S_+(\varepsilon, k_z) = S(\varepsilon, k_z) - \oint_\Gamma \frac{d\kappa}{v_\perp}[\varepsilon_{0\uparrow}(\mathbf{k}) - \varepsilon_0(\mathbf{k})]. \tag{13}$$

Insertion of the formula (13) into Eq. (12) gives the quantization condition (1) and the expression for the g factor:

$$g = -\frac{2m}{\pi m^*}\oint_\Gamma \frac{d\kappa}{v_\perp}\left[\mu_{0,11} + \frac{(\tau\mu_{0,12} + \tau^*\mu^*_{0,12})}{2}\right]. \tag{14}$$

Formulas (14), (8), and (9) permit one to find the g factor for any electron orbit. These formulas are equivalent to Eqs (52) and (64) of Roth's paper[7] and coincide with those of Ref. 5. Several formulas simplifying calculations of $\mu_{0,\rho\rho'}$ and $v_\perp$ in real situations are presented in the Appendix.

Since the g factor is the *measurable* quantity, formulas (8), (9), and (14) must be invariant under variations of phases of the Bloch factors $u_{\mathbf{k},l\rho}$ in spite of failing[32,37] this property for Hamiltonian (2). To prove this statement, consider the transformation,

$$u'_{\mathbf{k},01} = u_{\mathbf{k},01}\exp[i\phi(\mathbf{k})],$$

where $\phi(\mathbf{k})$ is some real function. According to the definition of $u_{\mathbf{k},02}$, we have, for $u_{\mathbf{k},02}$,

$$u'_{\mathbf{k},02} = u_{\mathbf{k},02}\exp[-i\phi(\mathbf{k})].$$

Then Eqs. (3)–(5) yield

$$\mu'_{0,11} = -\mu'_{0,22} = \mu_{0,11} - \mathbf{i}_z\left[\mathbf{v}_0 \times \frac{\partial\phi(\mathbf{k})}{\partial \mathbf{k}}\right],$$

$$\mu'_{0,12} = \mu_{0,12}\exp[-2i\phi(\mathbf{k})], \tag{15}$$

where $\mathbf{i}_z$ is the unit vector along $\mathbf{H}$. Using these equalities, it is easy to verify that a solution of the transformed equation (8), $\tau'(\mathbf{k})$, can be expressed through $\tau(\mathbf{k})$ as follows:

$$\tau'(\mathbf{k}) = \tau(\mathbf{k})\exp[2i\phi(\mathbf{k})]. \tag{16}$$

Taking into account Eqs. (15) and (16) and the relationship

$$\oint_\Gamma \frac{d\kappa}{v_\perp}\mathbf{i}_z\left[\mathbf{v}_0 \times \frac{\partial\phi(\mathbf{k})}{\partial \mathbf{k}}\right] = \oint_\Gamma d\mathbf{k}\frac{\partial\phi(\mathbf{k})}{\partial \mathbf{k}} = 0,$$

one obtains from formula (14) that g is invariant.

It is also instructive to find the g factor in the following case studied many years ago:[36] a small orbit Γ is located near the point $\mathbf{k}_{ex}$ of a minimum or a maximum of $\varepsilon_0(\mathbf{k})$. In this situation the quantities $\mu_{0,\rho\rho'}(\mathbf{k})$ calculated in the orbit are approximately constant, $\mu_{0,\rho\rho'}(\mathbf{k}) \approx \mu_{0,\rho\rho'}(\mathbf{k}_{ex})$, and Eq. (8) with condition (9) has the solutions

$$\tau = \frac{-\mu_{0,11} \pm \sqrt{(\mu_{0,11})^2 + |\mu_{0,12}|^2}}{\mu_{0,12}}, \tag{17}$$

where $\mu_{0,\rho\rho'} \equiv \mu_{0,\rho\rho'}(\mathbf{k}_{ex})$. Insertion of Eq. (17) into formula (14) yields the expression

$$g = \pm\frac{4m}{\hbar}\sqrt{(\mu_{0,11})^2 + |\mu_{0,12}|^2}, \tag{18}$$

which completely agrees with the appropriate formula of Ref. 36 if one takes into account that $\mathbf{v}_0(\mathbf{k}_{ex})=0$.

C. Analysis of other results

It is important to emphasize that Roth's result (14) has not been employed in the calculations of the g factor so far. The expression

$$g=\frac{2m}{\pi m^*}\oint_\Gamma \frac{d\kappa}{v_\perp}[-\mu_{0,11}(\mathbf{k})] \tag{19}$$

proposed by De Graaf and Overhauser[30] was used in numerous publications.[9–29] The discrepancy between formulas (14) and (19) is evident. It originates from the fact that De Graaf and Overhauser completely neglected the dynamics of the electron spin when they analyzed the semiclassical motion of the electron wave packet in the magnetic field. Besides this, it was stated in Ref. 30 that the concept of a local g factor $g(\mathbf{k})\propto\mu_{0,11}(\mathbf{k})$ can be defined. This concept was widely used in the g-factor calculations.[9–29] However, according to Eq. (14), only the g factor of the orbit has a physical meaning rather than the local g factors. Indeed, since τ is a solution of Eqs. (8) and (9), the value of this function at a point $\mathbf{k}$, $\tau(\mathbf{k})$, depends not only on the electron state of this point [i.e., on $\mu_{0,\rho\rho'}(\mathbf{k})$] but also on electron states of the whole *orbit* Γ [i.e., on $\mu_{0,\rho\rho'}(\mathbf{k}')$ at $\mathbf{k}'\neq\mathbf{k}$]. Thus, the same point of the Fermi surface can give different contributions to the g factors of different orbits passing through this point, and strictly speaking, the concept of the local g factor cannot be defined.

However, there is a case in which local g factors can be defined approximately. Both Eq. (14) and Eq. (19) lead to $g=2$ in the limit of a negligibly small spin-orbit interaction. Let us now evaluate the discrepancy between these formulas when the interaction remains weak but is not negligible. We shall describe the strength of the spin-orbit interaction in the crystal by the parameter

$$\nu\equiv\frac{\Delta}{E_0}\ll 1, \tag{20}$$

where Δ characterizes a shift of energy bands induced by ''turning on'' the interaction, while E_0 is a typical energy scale of an electron-band structure in the crystal (as a rule, E_0 is of the order of the atomic energies, $E_0\sim 0.1$–1 Ry). Then, we have $\mu^s_{0,11}\sim\hbar/2m$, $\mu^{or}_{0,11}\sim\mu_{0,12}\sim(\hbar/m)\nu$ (as to $\mu^{or}_{0,11}$; see also below), and Eqs. (8) and (9) yield

$$|\tau|\sim\oint_\Gamma|\mu_{0,12}|\frac{d\kappa}{v_\perp}\sim|\mu_{0,12}|\frac{m^*}{\hbar},$$

where we have used the well-known relation[2] $m^*=(\hbar/2\pi)\oint_\Gamma d\kappa/v_\perp$. It follows from these estimates that the discrepancy between formulas (14) and (19) is of the order of ν^2, while the correction to the free-electron value of g is of the first order in ν:

$$g-2=-\frac{2m}{\pi m^*}\oint_\Gamma\frac{d\kappa}{v_\perp}\mu^{or}_{0,11}\sim\nu.$$

Thus, when the spin-orbit interaction in the crystal is weak, the approach of De Graaf and Overhauser is sufficiently accurate, whereas in crystals with strong spin-orbit coupling, formulas (14), (8), and (9) are more suitable to calculate the g factor.

It was assumed in the estimates given above that $\Omega_{0\rho,0\rho'}\propto\nu$ at small ν. This is really true if there is no linking[5] of the electron orbit to band-contact lines which can exist in crystals.[38] But if the linking occurs and energies of the degenerate bands separate linearly in $\mathbf{k}$ in a vicinity of the band-contact line, one has:[37,5,6]

$$\oint_\Gamma\mathbf{\Omega}_{0\rho,0\rho}d\mathbf{k}=\pm\pi,$$

even for $\nu\to 0$. Then the first term in formula (4) for μ^{or} contributes to the g factor:

$$g-2\approx-\frac{2m}{\pi m^*}\oint_\Gamma\mathbf{\Omega}_{0\rho,0\rho}d\mathbf{k}=\mp\frac{2m}{m^*}.$$

In other words, we arrive at the following result: even though the spin-orbit coupling is very weak, the g factor can essentially differ from the free-electron value $g=2$ when the electron orbit links to the band-contact line.[5,6]

The linear muffin-tin orbital (LMTO) method[39] is frequently used to calculate electron energy bands of crystals. In the framework of this method local g factors of a number of metals were computed in Refs. 16–29. In those papers the following Hamiltonian of the electron in the magnetic field was used to find the g factors:

$$\hat{H}=\hat{H}_{LMTO}+HM^z, \tag{21}$$

where $\hat{H}_{LMTO}$ is the Hamiltonian of the electron in absence of the magnetic field written in the LMTO basis ($\hat{H}_{LMTO}$ includes the spin-orbit interaction here), while M^z is the electron magnetic moment calculated in this basis. Diagonalization of Hamiltonian (21) yields the energy bands and the magnetic moment M^z of the electron in the $\mathbf{k}$ representation. It was implied in Refs. 16–29 that this moment in the $\mathbf{k}$-representation just specifies the second term in Hamiltonian (2). However, according to Eq. (6), $M^z_{0,11}$ generally differs from $(e/c)\mu_{0,11}$. The difference appears in the process of diagonalizing $\hat{H}_{LMTO}$ since components of $\mathbf{k}$ are assumed to commute in the LMTO calculations. Thus, the approach based on Hamiltonian (21) can lead to inaccurate results for g factors even though the spin-orbit interaction is sufficiently weak and the concept of local g factors is a good approximation. In particular, it follows from Eq. (6) that one should exercise caution when $\mathbf{v}_0$ is not small in the orbit, i.e., when the energy band under study is not too narrow and the orbit does not lie near a point of a minimum or a maximum of $\varepsilon_0(\mathbf{k})$.

III. g FACTOR OF ZINC

As an example, we consider the g factor of zinc. The Brillouin zone of Zn is a hexagonal prism. Near the point K

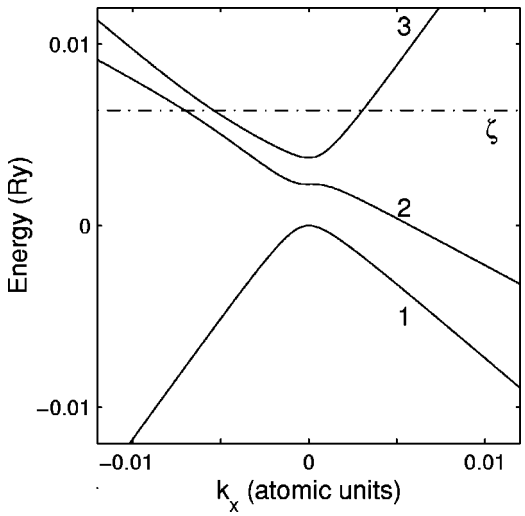

FIG. 1. Electron-energy bands of zinc in the vicinity of the point K at $k_y=k_z=0$. The coordinate k_x is directed along the line connecting the center of the Brillouin zone with the point K and is measured in the atomic units from this point. The figure is plotted for the case 2b of Table I (i.e., for one of the two possible sets of band parameters of zinc). The Fermi level ζ is indicated by the dash-dotted line.

lying in the middle of the vertical edge of the prism there are three bands which are close to each other and to the Fermi level ζ, Fig. 1. At the point K the symmetry types of these bands are K_7, K_8, and K_9,[33] and their energies at this point are equal to 0, $E_c+\Delta/3$, and $E_c-\Delta/3$, respectively (all energies are measured from the level K_7). The parameter E_c characterizes the crystal potential, while the quantity Δ is the spin-orbit constant which was estimated to be positive in zinc[33,35] (without the spin-orbit interaction the bands K_8 and K_9 would be degenerate at K). The Fermi level in zinc lies slightly above the bottom of the third (topmost) band at the point K. If $E_c<-\Delta/3$, the third band has symmetry type K_7, while if $E_c>-\Delta/3$, it has type K_8. The Fermi surface near the points K forms the so-called needles (they are long in the direction of the hexad axis which we denote as the z axis). In what follows we shall treat the electron orbits lying on the needles. We also assume that the magnetic field H is parallel to this z axis and $H<2.7$ kG; under this condition a probability of the magnetic breakdown between the needles and the second-band hole monster is negligible.[35]

The energy differences of importance for these bands are all less than 0.01 Ry (see Table I), while the nearest other bands at K lie about $E_0\simeq 0.4$ Ry away.[35] Thus, only the three-band **kp** Hamiltonian need be considered.[33] With account of spin components, the Hamiltonian matrix can be represented as follows:

$$\hat{\mathsf{H}}=\begin{pmatrix}\hat{\mathsf{H}}_1 & \hat{\mathsf{H}}_2\\ \hat{\mathsf{H}}_2^{+} & \hat{\mathsf{H}}_1'\end{pmatrix}, \tag{22}$$

where

TABLE I. Values of the band parameters used in the construction of Figs. 1 and 2.

Case	E_c (mRy)	Δ (mRy)	A (a.u.)	B (a.u.)
1a[a]	−2.3	2.1	0.66	0.76
1b	−2.3	2.1	0.76	0.66
2a	3.0	2.2	0.52	0.75
2b[b]	3.0	2.2	0.75	0.52
2c	3.0	2.2	0.60	0.60
3a	−0.7	2.1	0.66	0.76
3b	−0.7	2.1	0.76	0.66
3c	−0.7	2.1	0.71	0.71

[a]Case 2 of Ref. 35. $[\zeta-\varepsilon_3(0)]=2.7$ mRy.
[b]Case 3 of Ref. 35. $[\zeta-\varepsilon_3(0)]=2.6$ mRy.

$$\hat{\mathsf{H}}_1=\begin{pmatrix}0 & (A+C)k_- & (A-C)k_+\\ (A+C)k_+ & E_c+\dfrac{\Delta}{3} & Bk_-\\ (A-C)k_- & Bk_+ & E_c-\dfrac{\Delta}{3}\end{pmatrix}. \tag{23}$$

Here $\hat{\mathsf{H}}^{+}$ and $\hat{\mathsf{H}}'$ denote the Hermitian conjugate and transpose matrices, respectively; the origin of $\mathbf{k}$ is placed at the point K; k_x is directed along the line connecting the Brillouin-zone center and K; $k_\pm=k_x\pm ik_y$; A, B, and C are velocity matrix elements; $\mathsf{H}_{2,12}=-\mathsf{H}_{2,21}=2Ck_z$, and all other elements of matrix $\hat{\mathsf{H}}_2$ are equal to zero. The quantity C is the spin-orbit part of the velocity matrix elements. Its magnitude for zinc was evaluated[33] as $C=\hbar^2\Delta/6mA$. This leads to the estimates $C/A\sim C/B\sim\nu\sim 0.01$. The band energies $\varepsilon_l(\mathbf{k})$ $(l=1,2,3)$ are eigenvalues of the Hamiltonian and, according to Eqs. (22) and (23), are determined by the equation

$$-\varepsilon(D_+D_--B^2k_\perp^2)-\Lambda k_\perp^2+B(A^2-C^2)(k_+^3+k_-^3)-4C^2k_z^2D_-=0, \tag{24}$$

where $\Lambda=(A+C)^2D_-+(A-C)^2D_+$, $D_\pm=E_c\pm\Delta/3-\varepsilon$, and $k_\perp^2=k_-k_+$. Note also that the three-band model of the spectrum, Eqs. (22)–(24), is valid to the main order in the small parameter $\max(|E_c|,\Delta)/E_0\sim\nu$ (otherwise, other bands of zinc must be taken into account). In this context, one may put $C=0$ in Eq. (24).

In zinc the pure spin parts of $\mu_{0,\rho\rho'}$ are much less than the orbital components of these quantities, which is due to the small energy differences in the denominators of Eq. (4) (their relative magnitude is of the order of ν). Thus, it is allowed to completely neglect the pure spin contribution to the effective Hamiltonian. In this approximation and using Eq. (A7), we calculate the 2×2 Hermitian matrices $\hat{\mu}_l$ for each of the three bands $(l=1,2,3)$:

$$\frac{\mu_{l,11}}{v_\perp}=\frac{2}{|u|}\Bigg[2C^2B^2k_z^2D_-+(D_+D_-+2B^2k_\perp^2)\times\left(\frac{\Delta}{3}(A^2+C^2)-2AC(E_c-\varepsilon)\right)\Bigg], \quad (25)$$

$$\frac{\mu_{l,12}}{v_\perp}=\frac{4Ck_zB^2}{|u|}[2(A+C)D_-k_-+B(A-C)k_+^2], \quad (26)$$

where the complex quantity u is defined by the formula

$$u=2(D_+D_--B^2k_\perp^2)\{k_+(B^2\varepsilon-\Lambda)+3B(A^2-C^2)k_-^2\}.$$

With expressions (25) and (26), one can find the g factor for any of the three bands. Moreover, in the case of zinc, these formulas can be further simplified. Since Eqs. (22)–(24) are true to the main order in the parameter $\max(|E_c|,\Delta)/E_0$, it is justified to put $C=0$ in formulas (25) and (26). Then, we arrive at

$$\frac{\mu_{l,11}}{v_\perp}=\frac{2\Delta A^2}{3|u_0|}[D_+D_-+2B^2k_\perp^2], \quad \mu_{l,12}=0, \quad (27)$$

where $u_0\equiv u(C=0)$. Since $\mu_{l,12}=0$, Eq. (19) is applicable to calculate the g factor, and we obtain the formula

$$\delta_l(\varepsilon)\equiv\left.\frac{g_lm^*}{4m}\right|_{k_z=0}=-\left.\frac{1}{2\pi}\oint_{\Gamma^l}d\kappa\frac{\mu_{l,11}}{v_\perp}\right|_{k_z=0}, \quad (28)$$

for the quantity $\delta_l(\varepsilon)$ measured in the de Haas–van Alphen experiments. Note that δ_l are proportional to the small parameter Δ, which is in agreement with the estimates of Sec. II C. However, δ_l are not small in zinc since according to formulas (27) and (28), these quantities for the near-degenerate spectrum are determined by the ratio $\Delta/\max(|E_c|,|\zeta|)$ which of the order of unity in this metal, Table I.

Consider now the limiting case when the Fermi level lies near the topmost band edge [if $E_c<-\Delta/3$, this band is K_7, and its energy at the band edge is $\varepsilon_3(0)=0$; otherwise, this is K_8 and $\varepsilon_3(0)=E_c+\Delta/3$]. Then one obtains, from Eq. (28),

$$\delta_3=-\left.\frac{\mu_{3,11}m^*}{\hbar}\right|_{\mathbf{k}\to0},$$

where the formula for the cyclotron mass, $m^*=(\hbar/2\pi)\oint_\Gamma d\kappa/v_\perp$, has been used. In this limiting case the cyclotron mass is described by the expression

$$\frac{1}{m^*}=\frac{1}{\hbar^2}\left.\frac{2(\Lambda-\varepsilon_3(\mathbf{k})B^2)}{(\varepsilon_3(\mathbf{k})(D_++D-)-D_+D_-)}\right|_{\mathbf{k}=0},$$

while δ_3 is given by the formula

$$\delta_3=-\left|\left.\frac{\Delta A^2(D_+D_-+2B^2k_\perp^2)}{3(D_+D_--B^2k_\perp^2)(\Lambda-\varepsilon_3(\mathbf{k})B^2)}\right|_{\mathbf{k}\to0}\right|,$$

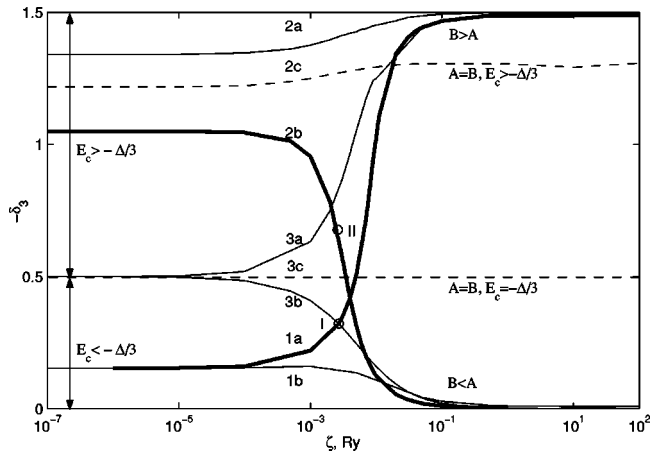

FIG. 2. The dependences $\delta_3(\zeta)$ for different values of the band parameters, Table I. Here the Fermi energy ζ is measured from the edge of the third band, $\varepsilon_3(0)$. Numbers near the curves indicate the cases in the Table I for which the curves are plotted (the curves with the number 1 correspond to $E_c<-\Delta/3$, while the curves 2 to $E_c>\Delta/3$; the case $A<B$ is described by the dependences 1a–3a, whereas the curves 1b–3b show the case $A>B$). The bold lines correspond to the possible sets of the band parameters of zinc (Ref. 35). At $A=B$, the dependences $\delta_3(\zeta)$ are shown by the dashed lines. In this case the limit value of δ_3 at large ζ depends on E_c/Δ [see Eq. (30)]. The circles mark the experimentally obtained pairs (ζ,δ_3) for zinc (Ref. 34).

where $\varepsilon_3(\mathbf{k})$ in $D_\pm$ and in Λ must be treated as $\varepsilon_3(\mathbf{k})\approx\varepsilon_3(0)+\hbar^2k_\perp^2/(2m^*)$. With the use of the Bennett-Falicov parameter $\xi=E_c/\Delta$, one eventually finds

$$\delta_3(\xi)=\begin{cases}\dfrac{1}{6\xi}, & \xi<-\dfrac{1}{3},\\ -1+\dfrac{2-(B/A)^2(3\xi+1)}{2[2+(B/A)^2(3\xi+1)]}, & \xi>-\dfrac{1}{3}.\end{cases} \quad (29)$$

If $E_c<-\Delta/3$, the expression (29) for δ_3 coincides with that of Bennett and Falicov[33] (corrected by Van Dyke *et al.*[35]), while in the case, $E_c>-\Delta/3$, it differs by -1 from the appropriate formula that follows from results of Ref. 33. Since in the semiclassical approach the change of δ by arbitrary integer do not affect the energy spectrum, we conclude that Eq. (29) agrees with the results of Bennett and Falikov. Note also that δ in Eq. (29) *continuously* decreases with ξ from 0 at $\xi=-\infty$ to $-3/2$ at $\xi=+\infty$.

The dependences of the quantity δ for the third band on the Fermi energy ζ are shown in Fig. 2. At $[\zeta-\varepsilon_3(0)]\to0$, the values of δ_3 agree with Eq. (29). In the high-energy limit $(\zeta\gg\Delta,|E_c|)$, the quantity $|\delta_3|$ always tends to 0 or to 3/2 if $A\neq B$, and the limiting value depends on a sign of $(\beta-1)$ where $\beta\equiv B/A$. In this context it should be noted that at $\zeta\gg\Delta$ the role of the spin-orbit interaction decreases, and one

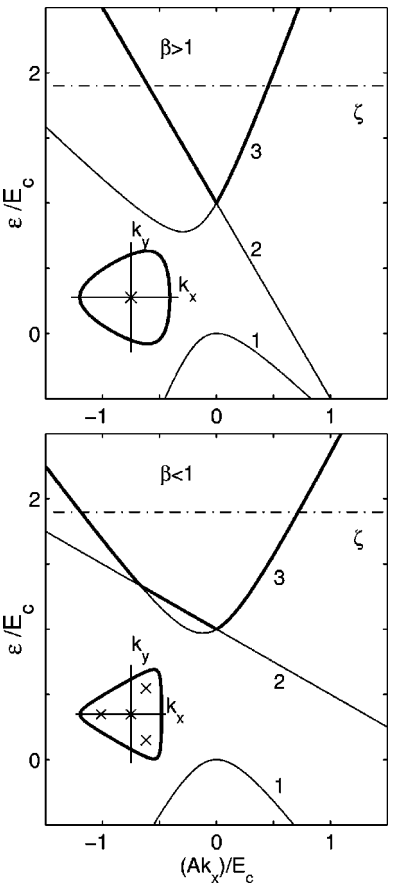

FIG. 3. The zinc-type band structure without the spin-orbit coupling ($\Delta=0$) at $k_y=k_z=0$. The upper and lower panels refer to the cases $B>A$ and $B<A$, respectively. The numbers mark the appropriate bands; the third band is indicated by the bold line. The dash-dotted lines represent the Fermi levels at which the semiclassical orbits in the third band are schematically shown in the insets. The crosses indicate the intersections of the band-contact lines with the plane $k_z=0$ (only the contact lines between the third and second bands are taken into account here; the lines are parallel to the z axis). Note that the semiclassical orbits are linked to one or four band-contact lines depending on the sign of $B-A$.

might expect to obtain $\delta\to 0$ in the high-energy limit. To clarify the unusual behavior of δ_3 presented in Fig. 2, let us put $\Delta\to 0$ and for definiteness assume that $E_c>0$. In this situation there are four band-contact lines in the vicinity of the point K; see Fig. 3. One of them is described by the equations, $k_x=k_y=0$, and in this line a contact of the second and the third bands occurs at the energy E_c. The other three lines intersect the plane $k_z=0$ at points which form a equilateral triangle with a center at point K. In these lines energies of the contacting bands are

$$E_{cont}=\frac{E_c}{1-\beta^2}.$$

If $\beta<1$ (i.e., $B<A$), a contact of the second and third bands occurs in the lines, while in the case $\beta>1$ the first and second bands contact there. It is also essential that the energies of the bands separate linearly in $\mathbf{k}$ in vicinities of all these four lines. According to the results of Refs. 5 and 6 (see also Sec. II C), if the orbit Γ surrounds such the contact lines between the band under study and some other one, then each of the lines contributes 1/2 (or $-1/2$) to the appropriate δ. When $\beta<1$, the orbit Γ at a sufficiently large ζ surrounds the *four* band-contact lines, and hence $\delta_3=0$. [Note that in the semiclassical approximation the integer part of δ has no effect on the spectrum since it can be absorbed by the number n in Eq. (1), and thus, any integer δ is equivalent to zero.] When $\beta>1$, there is only *one* contact line between the third and second bands inside the orbit Γ, and thus, δ_3 changes by 3/2 as compared with the case of $\beta<1$. In other words, the different limiting values of δ_3 in Fig. 2 are completely determined by the number of the band-contact lines which occur for the third band near the point K.

In the special case $A=B$, the high-energy limit of δ_3 depends on $\xi=E_c/\Delta$, Fig. 2. It can be shown that in this case the limiting value of δ_3 is given by the formula

$$\delta_3=-\frac{3}{4}-\frac{3}{2\pi}\arctan(\sqrt{3}\xi); \tag{30}$$

i.e., the value is not generally an integer or a half-integer. This is explained as follows: In the three-band model being investigated, the magnetic breakdown is absent when the inequality is met:

$$\{3[\xi\Delta+(1-\beta^2)\zeta]^2+\Delta^2\}\gg\frac{B^2|e|H}{\hbar c}. \tag{31}$$

(This inequality is written for $E_c,\Delta\ll\zeta$, $|\beta^2-1|\ll 1$.) If $\beta\neq 1$, one can put $\Delta=0$ in Eq. (30), and this condition is fulfilled due to the large value of ζ. However, if $\beta=1$, we cannot neglect the spin-orbit interaction, and the limiting value of δ_3 is not determined only by the number of the band-contact lines but also depends on the strength of the spin-orbit coupling. On the other hand, if $|E_c|=\Delta|\xi|\gg\Delta$ and the condition (31) is satisfied due to E_c, then it follows from Eq. (30) that δ_3 equals $-3/2$ ($E_c>0$) or 0 ($E_c<0$), which is in complete agreement with the considerations presented above.

Using data on the magnetoresistance and the de Haas–van Alphen effect, the two possible sets of values of the energy-band parameters for the needles in zinc were obtained[35]; see Table I. The existence of the two sets is due to the fact that only $|\delta|$ (up to an integer) can be found in experiments. After substitution of these two sets, our semiclassical formula leads to the values of $\delta_3(\zeta)$ coinciding with the experimental data,[34] Fig. 2. It is also worth noting that the dependences of $|\delta_3|$ on ζ are qualitatively different for these two sets of the parameters. This result may be useful in determining the energy-band parameters of zinc.

IV. CONCLUSIONS

The g factor appearing in the de Haas–van Alphen effect can be calculated using formulas (8), (9), and (14) (see also the Appendix). These formulas differ from Eq. (19) suggested by De Graaf and Overhauser.[30] The difference results from the following: when a Bloch electron moves in its

semiclassical orbit in an external magnetic field, a direction of the electron spin changes due to the spin-orbit interaction. De Graaf and Overhouser completely neglected this change, while Eqs. (8), (9), and (14) take it into account. Moreover, since the direction of the spin at a given point of the orbit depends on a prehistory of the electron motion, i.e., on characteristics of the orbit, the concept of the local g factor introduced in Ref. 30 is not, strictly speaking, correct. However, for a weak spin-orbit interaction in the crystal, the approaches lead to identical results for the g factor to the main order in the strength of the spin-orbit coupling (the discrepancy appears only in the next order). In this approximation the concept of the local g factor becomes valid.

As an example, we calculate the g factor for the three-band model of the electron spectrum, Eqs. (22), (23), and (24). This model is of interest in itself since it can describe the so-called electron needles in zinc. In this case the spin-orbit coupling is relatively small, and Eq. (19) is applicable to study the g factor for orbits lying on the needles. We analyze dependences of this g factor on the Fermi level ζ, Fig. 2. It is shown that g factor can essentially differ from zero even in the high-energy limit when ζ considerably exceeds gaps of the spectrum and the role of the spin-orbit interaction becomes negligible. In this case the so-called band-contact lines[38] give the main contribution to the g factor. This result is a manifestation of the general statement[5,6]: the g factor is determined not only by the strength of the spin-orbit coupling but also by band-contact lines linked to the semiclassical orbit. If we use values of the band parameters and ζ found in Ref. 35, our results for the g factor are in agreement with the experimental data for needles of zinc.[34]

APPENDIX: CALCULATION OF μ_0

Expressions (3)–(5) for $\hat{\mu}_0$ are written in the **k** representation, while other sets of basis functions are usually employed in electron-energy-band calculations. Besides this, the definition of $\mathbf{\Omega}_{\mathbf{n}\rho,\mathbf{m}\rho'}$, Eq. (5), includes the differentiation of wave functions. It is clear that the differentiation becomes a troublesome problem when the wave functions are found numerically. Here we point out the way of overcoming the above-mentioned problems: we derive expressions for $\hat{\mu}_0$, starting from representations widely used in practice, and show how to avoid the numerical differentiation.

Below we shall deal with only two sets of basis functions although our results can be applied to other representations with insignificant changes. The first set

$$\chi^{LK}_{\mathbf{k},l\rho}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{0,l\rho}(\mathbf{r})$$

corresponds to the Luttinger-Kohn representation (LKR).[40] Here the periodic factors $u_{\mathbf{k},l\rho}(\mathbf{r})$ of the Bloch functions are taken at a fixed point of the **k** space which we denote as zero. This basis is convenient for analytical calculation of $\varepsilon_0(\mathbf{k})$ and $\hat{\mu}_0(\mathbf{k})$ near the point $\mathbf{k}=0$ if several energy bands are close to $\varepsilon_0(\mathbf{k})$ in a vicinity of this point. In this situation small energy differences between the bands specify both $\varepsilon_0(\mathbf{k})$ and $\hat{\mu}_0(\mathbf{k})$ [see, e.g., Eq. (4)] and one can neglect all other bands.

The formulas given below are also applicable to the basis used in the LMTO method.[39] In this case the basis functions $\chi^{LMTO}_{\mathbf{k},l\rho}$ are Bloch sums of the muffin-tin orbitals. These functions, as well as $\chi^{LK}_{\mathbf{k},l\rho}$, possess the property of translation invariance,

$$\chi_{\mathbf{k},l\rho}(\mathbf{r}+\mathbf{a}) = e^{i\mathbf{k}\cdot\mathbf{a}} \chi_{\mathbf{k},l\rho}(\mathbf{r}),$$

where **a** is an arbitrary lattice vector and form the orthogonal and complete basis set (the orthogonality of $\chi^{LMTO}_{\mathbf{k},l\rho}$ can be always achieved by the well-known recursive procedure[39]). It is important that the **k** dependences of $\chi^{LMTO}_{\mathbf{k},l\rho}$ are determined by the so-called structure constants and thus are known for any type of lattice.

The Bloch functions $|\psi_{\mathbf{k},L}\rangle$ can be expressed through any of the above-mentioned sets as follows:

$$|\psi_{\mathbf{k},L}\rangle = \sum_M |\chi_{\mathbf{k},L}\rangle \mathsf{S}_{M,L}(\mathbf{k}),$$

where the capitals L and M denote couples of band and spinor indexes (e.g., $L \equiv \{l,\rho\}$), and matrix elements of the unitary transformation S are

$$\mathsf{S}_{M,L}(\mathbf{k}) = \langle \chi_{\mathbf{k},M} | \psi_{\mathbf{k},L} \rangle.$$

The transformation S diagonalizes a Hamiltonian matrix $\hat{\mathsf{H}}^{\chi}(\mathbf{k})$ of the electron in absence of the magnetic field in the χ representation (χ = LMTO or LK),

$$(\hat{\mathsf{S}}^{+}\hat{\mathsf{H}}^{\chi}\hat{\mathsf{S}})_{L,M} = \varepsilon_l(\mathbf{k})\,\delta_{L,M}. \tag{A1}$$

With the use of the matrix $\hat{\mathsf{S}}$, one can express $\hat{\mu}_0$ in Eq. (2) through quantities calculated in the χ representation:

$$\mu_{0,\rho\rho'} = (\hat{\mathsf{S}}^{+}\hat{\mathsf{R}}\hat{\mathsf{S}})_{0\rho,0\rho'} + \mathsf{Q}_{0,\rho\rho'}, \tag{A2}$$

$$\hat{\mathsf{R}} = \frac{1}{2}\left[\left(\hat{\Omega}^{\chi}_{y}\frac{\partial\hat{\mathsf{H}}^{\chi}}{\partial k_x} + \hat{v}^{\chi}_{x}\hat{\Omega}^{\chi}_{y}\right) - (x\leftrightarrow y)\right] + \hat{\mathsf{R}}^{s}, \tag{A3}$$

$$\mathsf{Q}_{0,\rho\rho'} = \frac{i}{2}\left[\hat{\mathsf{S}}^{+}\left(\frac{\partial\varepsilon_0}{\partial k_x} + \frac{\partial\hat{\mathsf{H}}^{\chi}}{\partial k_x}\right)\frac{\partial\hat{\mathsf{S}}}{\partial k_y} - (x\leftrightarrow y)\right]_{0\rho,0\rho'}. \tag{A4}$$

In these formulas the spin contribution $\hat{\mathsf{R}}^{s}$ and the matrix $\hat{\mathbf{\Omega}}^{\chi}$ are determined by Eqs. (3) and (5), respectively, with the spinors $u_{\mathbf{k},l\rho}$ replaced by $u^{\chi}_{\mathbf{k},l\rho} \equiv \exp(-i\mathbf{k}\mathbf{r})\chi_{\mathbf{k},l\rho}$; $\hat{\mathbf{v}}^{\chi}$ is the matrix of velocity in the χ representation. It is important to emphasize here that the **k** differentiations in $\hat{\mathbf{\Omega}}^{\chi}$ and in $\partial\hat{\mathsf{H}}^{\chi}\partial k_i$ can be now performed analytically since the **k** dependences of $\chi_{\mathbf{k},l\rho}$ are known both in the LKR and in the LMTO bases. However, in the LMTO method the matrix $\hat{\mathsf{S}}$ is found numerically, and thus the problem of calculating $\partial\hat{\mathsf{S}}/\partial k_i$ in Eq. (A4) appears. This problem can be resolved using the phase ambiguity of $\hat{\mu}_0$ discussed in Sec. II, and we

now obtain another formula for $\mathsf{Q}_{0,\rho\rho'}$ which enables one to avoid the numerical differentiations.

To calculate $\mathsf{Q}_{0,\rho\rho'}$, two columns in the matrix $\hat{\mathsf{S}}$ marked by indexes $\{l,\rho\}=\{0,1\},\{0,2\}$ are required. These columns are eigenvectors of the matrix $\hat{\mathsf{H}}^{\chi}$ corresponding to the eigenvalue $\varepsilon_0(\mathbf{k})$. If we denote these orthonormal vectors as $\vec{a}_0^{\rho}/|\vec{a}_0^{\rho}|$ with $\rho=1,2$, we arrive at the equation in $\vec{a}_0^{\rho}$,

$$[\hat{\mathsf{H}}^{\chi}(\mathbf{k})-\varepsilon_0(\mathbf{k})]\vec{a}_0^{\rho}(\mathbf{k})=0 \tag{A5}$$

(note that we do not assume $|\vec{a}_0^{\rho}|=1$ here). To proceed further, let us represent $\hat{\mathsf{H}}^{\chi}$ in the block form

$$\hat{\mathsf{H}}^{\chi}_{2N\times 2N}=\begin{pmatrix} E_0(\mathbf{k})\hat{\mathbb{1}}_{2\times 2} & \hat{V}_{2\times(2N-2)}(\mathbf{k}) \\ \hat{V}^{+}_{(2N-2)\times 2}(\mathbf{k}) & \hat{M}_{(2N-2)\times(2N-2)}(\mathbf{k}) \end{pmatrix},$$

where $E_0(\mathbf{k})$ is a scalar function, and the subscripts indicate dimensions of some matrix $\hat{V}$ and $\hat{M}$. Construct two $2N$-dimensional vectors $\vec{a}^{\rho}$ $(\rho=1,2)$ as follows:

$$\vec{a}^{\rho}(\mathbf{k},E)=\det(\hat{M}-E)\begin{pmatrix} e^{(\rho)} \\ -(\hat{M}-E)^{-1}\hat{V}^{+}e^{(\rho)} \end{pmatrix}. \tag{A6}$$

Here

$$e^{(1)}=\begin{pmatrix}1\\0\end{pmatrix},\quad e^{(2)}=\begin{pmatrix}0\\1\end{pmatrix},$$

and N is the number of the electron bands that are allowed for the computation. It is follows from formula (A6) that components of the vectors $\vec{a}^{\rho}(\mathbf{k},E)$ are polynomials of $\mathsf{H}^{\chi}_{ij}(\mathbf{k})$ and E. If the parameter E is substituted by $\varepsilon_0(\mathbf{k})$, the vector $\vec{a}^{\rho}$ reduces to the eigenvector $\vec{a}_0^{\rho}$, Eq. (A5). It can be shown that the quantity $\mathsf{Q}_{0,\rho\rho'}$, Eq. (A4), can be found from the relation

$$\mathsf{Q}_{0,\rho\rho'}(\mathbf{k})=\mathsf{Q}_{0,\rho\rho'}(\mathbf{k},E=\varepsilon_0(\mathbf{k})),$$

where

$$\mathsf{Q}_{0,\rho\rho'}(\mathbf{k},E)=\frac{i}{2|\vec{a}^{\rho}(E,\mathbf{k})|^2}\times\left\{\left(\frac{\partial\vec{a}^{\rho}(E,\mathbf{k})}{\partial k_y},[\hat{\mathsf{H}}^{\chi}(\mathbf{k})-E]\frac{\partial\vec{a}^{\rho'}(E,\mathbf{k})}{\partial k_x}\right)-(x\leftrightarrow y)\right\} \tag{A7}$$

is the function of *two independent* variables E and $\mathbf{k}$ [i.e., E is not differentiated with respect to $\mathbf{k}$ in Eq. (A7)]. Here $(\vec{a},\hat{A}\vec{b})\equiv\Sigma_{ij}a_i^{*}A_{ij}b_j$ for any matrix $\hat{A}$ and vectors $\vec{a}$ and $\vec{b}$. Thus, $\mathsf{Q}_{0,\rho\rho'}$ can be expressed through matrix elements of $\hat{\mathsf{H}}^{\chi}$ and their derivatives with respect to $\mathbf{k}$. Since in the LMTO representation the $\mathbf{k}$ dependences of these matrix elements are determined by structure constants[39] and the above-mentioned derivatives can be calculated analytically, Eq. (A7) enables one to avoid numerical differentiations of $\hat{\mathsf{S}}(\mathbf{k})$ [in principle, with Eqs. (A2), (A3), and (A7) the calculation of $\mu_{0,\rho\rho'}(\mathbf{k})$ by the LMTO method is not more complicated than the computation of $\varepsilon_0(\mathbf{k})$]. Interestingly, formula (A7) also simplifies calculations in the LKR. In this representation the elements of $\hat{\mathsf{H}}^{\chi}$ have simple dependences on $\mathbf{k}$, while $\hat{\mathbf{\Omega}}^{LK}=0$ (and thus $\hat{R}$ coincides with the spin contribution $\hat{R}^{s}$, the latter being relatively small when $m_c\ll m$). It is also worth noting that $v_{\perp}$ entering Eqs. (8) and (14) can be found using the formula $(i=x,y)$

$$v_i=\frac{1}{|\vec{a}_0^{\rho}|^2}\left(\vec{a}_0^{\rho},\frac{\partial\hat{\mathsf{H}}^{\chi}}{\partial k_i}\vec{a}_0^{\rho}\right). \tag{A8}$$

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