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Effect of nonparabolicity on the conduction-electron spin resonance in cubic semiconductors

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The spin-resonance amplitude of conduction electrons in a cubic crystal has been calculated keeping terms up to fourth order in the wave vector $\mathbf{k}$ in the 2×2 effective-mass Hamiltonian. Apart from corrections to the magnetic dipole amplitude, we find that the terms $\gamma_0\mu_B(\sigma_x B_{0x}k_x^2+\sigma_y B_{0y}k_y^2+\sigma_z B_{0z}k_z^2)$ and $g''\mu_B\{\boldsymbol{\sigma}\cdot\mathbf{k},\mathbf{B}_0\cdot\mathbf{k}\}$ yield electric dipole amplitudes proportional to $\mathbf{k}\cdot\mathbf{B}_0$. While in the ordinary Voigt and cyclotron-resonance-active Faraday configurations only the γ_0 term is effective, in the cyclotron-resonance-inactive Faraday configuration both the γ_0 and g'' terms contribute. We have calculated the angular dependence of the γ_0 amplitude for arbitrary crystal orientations, the g'' amplitude being isotropic. In narrow-band-gap materials the admixture of hole states into the electron eigenstates also contributes an isotropic electric dipole spin-flip amplitude proportional to $\mathbf{k}\cdot\mathbf{B}_0$, which is distinct from those mentioned.

I. INTRODUCTION

In the presence of a magnetic field $\mathbf{B}_0=\nabla\times\mathbf{A}_0$, the electrons in an orbitally nondegenerate band of a cubic crystal in which the energy minimum occurs at the center of the first Brillouin zone are described, in the lowest approximation, by the Hamiltonian

$$H_0=\frac{1}{2m^*}\left[\mathbf{p}+\frac{e}{c}\mathbf{A}_0\right]^2+\tfrac{1}{2}g_0\mu_B\boldsymbol{\sigma}\cdot\mathbf{B}_0\ , \tag{1}$$

where m^* and g_0 are the effective mass and g factor, respectively. The eigenvalues of H_0 are the Landau levels

$$E_n^{(s)}(k_\zeta)=\hbar\omega_c(n+\tfrac{1}{2})+\frac{\hbar^2k_\zeta^2}{2m^*}+g_0\mu_B B_0 s\ , \tag{2}$$

where $\omega_c=eB_0/m^*c$ is the cyclotron frequency, n is the Landau principal quantum number ($n=0,1,2,\ldots$), and $\hbar k_\zeta$ and s are the eigenvalues of the components of $\mathbf{p}$ and $\frac{1}{2}\boldsymbol{\sigma}$ along the direction of $\mathbf{B}_0$. The corresponding eigenstates can be written in the following factorized form,[1]

$$\phi(n,n_b,k_\zeta,s)=\phi_{nn_b}(2\pi)^{-1/2}\exp(ik_\zeta\zeta)\chi_s\ , \tag{3}$$

where ϕ_{nn_b} refers to the orbital motion in the plane perpendicular to $\mathbf{B}_0$, $(2\pi)^{-1/2}\exp(ik_\zeta\zeta)$ to the orbital motion along the direction of $\mathbf{B}_0$, and χ_s describes the spin state; these eigenstates are highly degenerate with respect to the quantum number n_b ($n_b=0,1,2,\ldots$); since n_b is immaterial for our purposes, from now on it will be ignored.

Here, we are mainly interested in the spin-flip resonance at energy $\hbar\omega_s=g_0\mu_B B_0$ corresponding to transitions in which the spin s is reversed while the principal quantum number n remains unchanged.[2] The spin resonance is electric dipole forbidden in the approximation of Eq. (1), but becomes allowed and is called electric dipole spin resonance (EDSR) when either higher-order terms are included in H_0 or the mixing of states from nearby bands into the electron eigenstates is taken into account. Even though these two corrections are due to the same physical reason, i.e., the interaction with other bands, they are quite distinct, as will be shown later. Of course, it is also possible to resort to a multiband approach in which conduction and valence bands are treated on the same footing. However, the latter theoretical framework always requires a good deal of numerical calculations and is often not very transparent. Therefore, as long as only intraband transitions are of interest, a reduction to a single-band scheme, which allows one to perform analytical calculations, is desirable.

Including terms up to fourth order in the wave vector $\mathbf{k}$ [$\hbar\mathbf{k}=\mathbf{p}+(e/c)\mathbf{A}_0$], the 2×2 electron Hamiltonian is[3,4]

$$H=H_0+H_A+H_C\ , \tag{4}$$

where H_0 is given by Eq. (1) and

$$\begin{aligned}H_A&=\delta_0\boldsymbol{\sigma}\cdot\boldsymbol{\kappa}\ ,\\ H_C&=\epsilon_0k^4+\alpha_0(\{k_x^2,k_y^2\}+\{k_y^2,k_z^2\}+\{k_z^2,k_x^2\})+\beta_0\mu_B^2B_0^2+g'\mu_B\boldsymbol{\sigma}\cdot\mathbf{B}_0k^2+g''\mu_B\{\boldsymbol{\sigma}\cdot\mathbf{k},\mathbf{B}_0\cdot\mathbf{k}\}\\ &\quad+\gamma_0\mu_B(\sigma_xB_{0x}k_x^2+\sigma_yB_{0y}k_y^2+\sigma_zB_{0z}k_z^2)\ ;\end{aligned} \tag{5}$$

the curly brackets represent the quantum-mechanical anticommutator. Here, the operators κ_x, κ_y, and κ_z are

$$\begin{aligned}\kappa_x&=k_yk_xk_y-k_zk_xk_z\ ,\\ \kappa_y&=k_zk_yk_z-k_xk_yk_x\ ,\\ \kappa_z&=k_xk_zk_x-k_yk_zk_y\ ,\end{aligned}\tag{6}$$

and the parameters δ_0, ϵ_0, α_0, β_0, g', g'', and γ_0 are material constants which can either be taken from experiments or calculated within $\mathbf{k}\cdot\mathbf{p}$ perturbation models of various degrees of sophistication.[4–6] We note that H_A is odd under inversion, while H_C is even; the latter has O_h point-group symmetry, while the former only T_d symmetry, which is appropriate for binary compounds such as InSb and GaAs. In first-order perturbation theory[7] it is easy to see how H_A and H_C bring about electric dipole spin-flip transition matrix elements because of the presence of the spin-orbit–coupling terms proportional to δ_0, g'', and γ_0.[8] While the term in δ_0, which is odd, gives an even, effective, electric-dipole operator that can induce spin-flip transitions between eigenstates of H_0 with $k_\zeta=0$, the terms in g'' and γ_0 give an odd electric dipole operator that can induce spin-flip transitions only between eigenstates with $k_\zeta\neq0$, which do not have a definite parity. Furthermore, the terms in g', g'', and γ_0 modify the g tensor and thus both the spin-resonance energy $\hbar\omega_s$ and the magnetic dipole transition matrix element. The EDSR amplitude induced by H_A and H_C and the complete magnetic dipole amplitude are calculated in Sec. II.

An additional contribution to the electric dipole spin resonance, as we said, comes not from complications of the conduction-band dispersion relation, but from the admixture of, say, hole wave functions into the conduction-electron eigenstates. This effect, which can be important in narrow-band-gap materials, is discussed in Sec. III on the basis of a very simple three-band model for InSb.[9] As this model calculation neglects inversion symmetry-breaking terms (they are, in this context, a second-order effect), the resulting transition amplitude is proportional to k_ζ, just as that caused by H_C. Finally, in Sec. IV, we give a few numerical estimates for InSb and GaAs.

II. ELECTRON-SPIN-RESONANCE AMPLITUDE

In the present section,[10] we give the spin-flip transition-matrix elements for arbitrary experimental configurations. H_A and H_C are treated as perturbations to H_0; the perturbed eigenstates are expressed as

$$|\psi_\nu\rangle=e^{iS}|\nu\rangle\ ,\tag{7}$$

here $|\nu\rangle=|n,k_\zeta,s\rangle$ are the eigenstates of H_0 and the Hermitian operator S is such that $e^{-iS}He^{iS}$ is diagonal in the unperturbed representation, i.e.,

$$e^{-iS}He^{iS}|\nu\rangle=E(\nu)|\nu\rangle\ ,\tag{8}$$

where the symbols $E(\nu)$ represent the perturbed energies. To first order in H_A and H_C, S is given by[11]

$$S\simeq S_A+S_C\ ,\tag{9}$$

with

$$H_A+i[H_0,S_A]=0\ ,\tag{10}$$

and

$$H_C+i[H_0,S_C]=0\ ,\tag{11}$$

where the square brackets denote commutators. Under the action of a radiation field described as a plane wave of frequency ω, polarization $\hat{\varepsilon}$ and wave vector $\mathbf{q}=\sqrt{\epsilon}(\omega/c)\hat{\mathbf{n}}$ (ϵ is the dielectric constant), the transition amplitude is proportional to

$$M_{\nu'\nu}=\langle\psi_{\nu'}|V|\psi_\nu\rangle\simeq\langle\nu'|V+i[V,S]|\nu\rangle\ ,\tag{12}$$

with

$$V=\tfrac{1}{2}\{\hat{\varepsilon}\cdot\mathbf{v},e^{i\mathbf{q}\cdot\mathbf{r}}\}+\frac{i\hbar\omega}{8mc}\sqrt{\epsilon}\{(\hat{\mathbf{n}}\times\hat{\varepsilon})\cdot\underset{\sim}{g}\cdot\boldsymbol{\sigma},e^{i\mathbf{q}\cdot\mathbf{r}}\}\ ,\tag{13}$$

where the g tensor is defined by

$$\frac{\partial H}{\partial\mathbf{B}_0}=\tfrac{1}{2}\mu_B\underset{\sim}{g}\cdot\boldsymbol{\sigma}\tag{14}$$

and the velocity operator $\mathbf{v}=(1/i\hbar)[\mathbf{r},H]$ is the sum of three terms $\mathbf{v}_0$, $\mathbf{v}_A$, and $\mathbf{v}_C$ corresponding to each of the three parts of the Hamiltonian H_0, H_A, and H_C. Disregarding the spatial dependence of the incoming radiation, the first term in Eq. (13) gives the electric dipole amplitude, while the second gives the magnetic dipole amplitude.

To calculate transition matrix elements, the expressions of H_A and H_C with respect to the ξ,η,ζ axes ($\hat{\zeta}\|\mathbf{B}_0$) are needed, H_0 being isotropic. To obtain these we use the Euler angles of the triad $(\hat{\xi},\hat{\eta},\hat{\zeta})$ with respect to the cubic axes $(\hat{\mathbf{x}},\hat{\mathbf{y}},\hat{\mathbf{z}})$. The Euler angles are defined as follows.

(i) α is the angle between $\hat{\mathbf{y}}$ and the line of nodes $\hat{\mathbf{z}}\times\hat{\zeta}$.
(ii) β is the angle formed by $\hat{\mathbf{z}}$ and $\hat{\zeta}$.
(iii) γ is the angle between the (ξ,ζ) and (ζ,z) planes. Clearly, $0\le\alpha<2\pi$, $0\le\beta\le\pi$, and $0\le\gamma<2\pi$.

For any vector $\mathbf{u}$,

$$u_i=\sum_\kappa u_\kappa R_{i\kappa}\ ,\tag{15}$$

where $i=x,y,z$, $\kappa=+,-,\zeta$, and

$$u_\pm=u_\xi\pm iu_\eta\ .\tag{16}$$

The coefficients $R_{i\kappa}$ are given by

$$\begin{aligned}R_{x,+}&=R^*_{x,-}=\tfrac{1}{2}e^{i\gamma}(\cos\alpha\cos\beta+i\sin\alpha)\ ,\\ R_{x\zeta}&=\cos\alpha\sin\beta\ ,\\ R_{y,+}&=R^*_{y,-}=\tfrac{1}{2}e^{i\gamma}(\sin\alpha\cos\beta-i\cos\alpha)\ ,\\ R_{y\zeta}&=\sin\alpha\sin\beta\ ,\\ R_{z,+}&=R^*_{z,-}=-\tfrac{1}{2}e^{i\gamma}\sin\beta\ ,\\ R_{z\zeta}&=\cos\beta\ .\end{aligned}\tag{17}$$

The form of H_A is

$$H_A=\tfrac{1}{2}\delta_0 \sum_{\kappa,\lambda,\mu,\nu} \sigma_\kappa\{k_\lambda, k_\mu k_\nu\}(\kappa\lambda;\mu\nu) , \tag{18}$$

where the symbols $(\kappa\lambda;\mu\nu)$ are given by

$$(\kappa\lambda;\mu\nu)= \sum_{k,i,j} \varepsilon_{kij}R_{i\kappa}R_{i\lambda}R_{j\mu}R_{j\nu} \tag{19}$$

and ε_{kij} is the Levi-Cività rank-3 completely antisymmetric tensor density. H_A is conveniently expressed in terms of the four functions

$$F_0=-\frac{3i}{16}\sin(2\alpha)\sin(2\beta)\sin\beta , \tag{20}$$

$$F_1=\tfrac{1}{16}e^{i\gamma}[\cos(2\alpha)\sin(2\beta)+i \sin(2\alpha)\sin\beta(3\cos^2\beta-1)] , \tag{21}$$

$$F_2=\tfrac{1}{16}e^{2i\gamma}[2 \cos(2\alpha)\cos(2\beta) +i \sin(2\alpha)\cos\beta(3\cos^2\beta-1)] , \tag{22}$$

and

$$F_3=\tfrac{3}{16}e^{3i\gamma}[\cos(2\alpha)\sin(2\beta)+i \sin(2\alpha)\sin\beta(1+\cos^2\beta)] , \tag{23}$$

as

$$H_A=\tfrac{1}{2}\delta_0(\sigma_\xi+i\sigma_\eta)\Omega+\tfrac{1}{2}\delta_0(\sigma_\xi-i\sigma_\eta)\Omega^\dagger+\delta_0\sigma_\zeta\Omega_\zeta , \tag{24}$$

where

$$\begin{aligned}\Omega= {}&(k_+k_-^2+k_-^2k_+-8k_-k_\zeta^2)F_0\\ &+2(3k_+k_-k_\zeta+3k_-k_+k_\zeta-4k_\zeta^3)F_1\\ &+2(k_+k_-k_+-4k_+k_\zeta^2)F_2+2k_+^2k_\zeta F_3\\ &-10k_-^2k_\zeta F_1^*-2k_-^3F_2^*\end{aligned} \tag{25}$$

and

$$\Omega_\zeta=[(k_+k_-k_+-k_+^2k_--k_-k_+^2 +4k_+k_\zeta^2)F_1+4k_+^2k_\zeta F_2-k_+^3F_3]+\text{H.c.} \tag{26}$$

The terms proportional to ϵ_0, α_0, β_0, and g' do not contribute to the spin-flip amplitude. The remaining terms of H_C are

$$g''\mu_B\{\sigma\cdot\mathbf{k}, \mathbf{B}_0\cdot\mathbf{k}\}=2g''\mu_B B_0 k_\zeta[\sigma_\zeta k_\zeta+\tfrac{1}{2}(\sigma_\xi+i\sigma_\eta)k_-+\tfrac{1}{2}(\sigma_\xi-i\sigma_\eta)k_+] \tag{27}$$

and

$$\gamma_0\mu_B\sum_i B_{0i}\sigma_i k_i^2=\gamma_0\mu_B B_0 \sum_{\tau,\mu,\nu}\sigma_\tau k_\mu k_\nu \sum_i R_{i\zeta}R_{i\tau}R_{i\mu}R_{i\nu} . \tag{28}$$

The tensor $\underset{\sim}{g}$ is given by

$$\underset{\sim}{g}=(g_0+2g'k^2)\underset{\sim}{1}+2g''\{\mathbf{k},\mathbf{k}\}+2\gamma_0(\hat{\mathbf{x}}\hat{\mathbf{x}}k_x^2+\hat{\mathbf{y}}\hat{\mathbf{y}}k_y^2+\hat{\mathbf{z}}\hat{\mathbf{z}}k_z^2) , \tag{29}$$

which contains an anisotropic part proportional to γ_0, namely

$$2\gamma_0\sum_i k_i^2\hat{\mathbf{r}}_i\hat{\mathbf{r}}_i=2\gamma_0\sum_{\lambda,\mu,\nu,\rho}k_\lambda k_\mu\hat{\mathbf{r}}_\nu\hat{\mathbf{r}}_\rho\sum_i R_{i\lambda}R_{i\mu}R_{i\nu}R_{i\rho} . \tag{30}$$

While in the magnetic dipole amplitude different combinations of the components of $\underset{\sim}{g}$ might be involved, depending on the experimental configuration, the spin-resonance frequency ω_s, depending only on $\underset{\sim}{g}_{\zeta\zeta}$, is[12]

$$\hbar\omega_s=\mu_B B_0|\langle n,k_\zeta|g_{\zeta\zeta}|n,k_\zeta\rangle|=\mu_B B_0\left|g_0+2g'\left[\frac{1}{R_0^2}(2n+1)+k_\zeta^2\right]+4g''k_\zeta^2 +2\gamma_0\left[\frac{2}{R_0^2}(2n+1)\sum_i R_{i+}R_{i-}R_{i\zeta}^2+k_\zeta^2\sum_i R_{i\zeta}^4\right]\right| , \tag{31}$$

where $|n,k_\zeta\rangle$ represents the orbital part of the Landau eigenstate; the absolute value is needed for materials with a negative g factor (like InSb and GaAs).

We now proceed to evaluate the spin-resonance amplitude $M_{\nu'\nu}$ in both the Voigt and Faraday configurations for arbitrary crystal orientations. In the Voigt configurations, taking $\hat{\mathbf{n}}=\hat{\eta}$, we can neglect the spatial dependence of the incident radiation field $e^{iq\eta}$ and consider as initial and final states $|n,k_\zeta,\frac{1}{2}\rangle$ and $|n,k_\zeta,-\frac{1}{2}\rangle$, respectively. In the ordinary Voigt (OV) configuration $\hat{\varepsilon}=\hat{\xi}$ and

$$V=v_{0\zeta}+v_{A\zeta}+v_{C\zeta}+\frac{i\hbar\omega}{4mc}\sqrt{\epsilon}\hat{\xi}\cdot\underset{\sim}{g}\cdot\sigma ; \tag{32}$$

we have

$$\langle n,k_\zeta,-\tfrac{1}{2}|v_{0\zeta}|n,k_\zeta,\tfrac{1}{2}\rangle=\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{\hbar k_\zeta}{m^*}\right|n,k_\zeta,\frac{1}{2}\right\rangle=0 , \tag{33}$$

$$\langle n,k_\zeta,-\tfrac{1}{2}|v_{A\zeta}|n,k_\zeta,\tfrac{1}{2}\rangle=\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{1}{\hbar}\frac{\partial H_A}{\partial k_\zeta}\right|n,k_\zeta,\frac{1}{2}\right\rangle=\frac{\delta_0}{\hbar}\left\langle n,k_\zeta\left|\frac{\partial\Omega^\dagger}{\partial k_\zeta}\right|n,k_\zeta\right\rangle=\frac{24\delta_0}{\hbar R_0^2}(n+\tfrac{1}{2}-k_\zeta^2R_0^2)F_1^* \ , \tag{34}$$

and

$$\langle n,k_\zeta,-\tfrac{1}{2}|v_{C\zeta}|n,k_\zeta,\tfrac{1}{2}\rangle=\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{1}{\hbar}\frac{\partial H_C}{\partial k_\zeta}\right|n,k_\zeta,\frac{1}{2}\right\rangle=\frac{\gamma_0\mu_B B_0}{\hbar}4k_\zeta\sum_i R_{i\zeta}^3R_{i-} \ , \tag{35}$$

Then, as S is already of first order in H_A and H_C, we have

$$\langle n,k_\zeta,-\tfrac{1}{2}|i[V,S]|n,k_\zeta,\tfrac{1}{2}\rangle\simeq\langle n,k_\zeta,-\tfrac{1}{2}|i[v_{0\zeta},S]|n,k_\zeta,\tfrac{1}{2}\rangle=\frac{i\hbar}{m^*}(k_\zeta-k_\zeta)\langle n,k_\zeta,-\tfrac{1}{2}|S|n,k_\zeta,\tfrac{1}{2}\rangle=0 \ . \tag{36}$$

Finally, the magnetic dipole term is

$$\begin{aligned}\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{i\hbar\omega}{4mc}\sqrt{\epsilon}\hat{\xi}\cdot\underset{\sim}{g}\cdot\sigma\right|n,k_\zeta,\frac{1}{2}\right\rangle&=\frac{i\hbar\omega}{4mc}\sqrt{\epsilon}\langle n,k_\zeta|\hat{\xi}\cdot\underset{\sim}{g}\cdot(\hat{\xi}+i\hat{\eta})|n,k_\zeta\rangle\\&=\frac{i\hbar\omega}{4mc}\sqrt{\epsilon}\langle n,k_\zeta|g_0+2g'k^2+2g''k_\xi k_++2g''k_+k_\xi\\&\quad+4\gamma_0\sum_{\mu,\nu}k_\mu k_\nu\sum_i(R_{i+}+R_{i-})R_{i-}R_{i\mu}R_{i\nu}|n,k_\zeta\rangle\\&\equiv\frac{i\hbar\omega}{4mc}\sqrt{\epsilon}g_{\rm OV}(n,k_\zeta) \ ,\end{aligned} \tag{37}$$

where

$$\begin{aligned}g_{\rm OV}(n,k_\zeta)=g_0&+\frac{2g'}{R_0^2}(2n+1+k_\zeta^2R_0^2)+\frac{4g''}{R_0^2}(n+\tfrac{1}{2})+4\gamma_0k_\zeta^2\sum_i(R_{i+}+R_{i-})R_{i-}R_{i\zeta}^2\\&+\frac{8\gamma_0}{R_0^2}(2n+1)\sum_i(R_{i+}+R_{i-})R_{i+}R_{i-}^2 \ .\end{aligned} \tag{38}$$

Hence, for the OV configuration, we obtain

$$\begin{aligned}M_{v'v}&\simeq\langle n,k_\zeta,-\tfrac{1}{2}|(V+i[V,S])|n,k_\zeta,+\tfrac{1}{2}\rangle\\&\simeq\frac{12\delta_0}{\hbar R_0^2}\left[(2n+1-2k_\zeta^2R_0^2)F_1^*+\frac{\hbar^2k_\zeta\gamma_0}{6m\delta_0}\sum_i R_{i-}R_{i\zeta}^3\right]+\frac{i\hbar\omega}{4mc}\sqrt{\epsilon}g_{\rm OV}(n,k_\zeta) \ ,\end{aligned} \tag{39}$$

In the extraordinary Voigt (EV) configuration, with $\hat{\mathbf{n}}=\hat{\eta}$ and $\hat{\boldsymbol{\varepsilon}}=\hat{\xi}$, we have

$$V=v_{0\xi}+v_{A\xi}+v_{C\xi}-\frac{i\hbar\omega}{4mc}\sqrt{\epsilon}\hat{\zeta}\cdot\underset{\sim}{g}\cdot\sigma \tag{40}$$

and

$$\langle n,k_\zeta,-\tfrac{1}{2}|v_{0\xi}|n,k_\zeta,\tfrac{1}{2}\rangle=\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{\hbar k_\xi}{m^*}\right|n,k_\zeta,\frac{1}{2}\right\rangle=0 \ , \tag{41}$$

$$\begin{aligned}\langle n,k_\zeta,-\tfrac{1}{2}|v_{A\xi}|n,k_\zeta,\tfrac{1}{2}\rangle&=\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{1}{\hbar}\frac{\partial H_A}{\partial k_\xi}\right|n,k_\zeta,\frac{1}{2}\right\rangle\\&=\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{1}{\hbar}\left[\frac{\partial H_A}{\partial k_+}+\frac{\partial H_A}{\partial k_-}\right]\right|n,k_\zeta,\frac{1}{2}\right\rangle\\&=\frac{\delta_0}{\hbar}\left\langle n,k_\zeta\left|\frac{\partial\Omega^\dagger}{\partial k_+}+\frac{\partial\Omega^\dagger}{\partial k_-}\right|n,k_\zeta\right\rangle\\&=\frac{4\delta_0}{\hbar R_0^2}(F_0^*+F_2^*)(2n+1-2k_\zeta^2R_0^2) \ ,\end{aligned} \tag{42}$$

and

$$\langle n,k_\zeta,-\tfrac{1}{2}|v_{C\xi}|n,k_\zeta,+\tfrac{1}{2}\rangle=\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{1}{\hbar}\left[\frac{\partial H_C}{\partial k_+}+\frac{\partial H_C}{\partial k_-}\right]\right|n,k_\zeta,\frac{1}{2}\right\rangle$$
$$=\frac{2g''\mu_B B_0}{\hbar}k_\zeta+\frac{4\gamma_0\mu_B B_0}{\hbar}k_\zeta\sum_i R_{i\zeta}^2 R_{i-}(R_{i+}+R_{i-})\ . \tag{43}$$

Then, we have

$$\langle n,k_\zeta,-\tfrac{1}{2}|i[V,S]|n,k_\zeta,\tfrac{1}{2}\rangle\simeq\left\langle n,k_\zeta,-\frac{1}{2}\left|i\frac{\hbar}{m^*}[k_\xi,S]\right|n,k_\zeta,\frac{1}{2}\right\rangle$$
$$=i\frac{\hbar}{m^*}\sum_{l=n\pm1}(\langle n,k_\zeta,-\tfrac{1}{2}|k_\xi|l,k_\zeta,-\tfrac{1}{2}\rangle\langle l,k_\zeta,-\tfrac{1}{2}|S|n,k_\zeta,\tfrac{1}{2}\rangle$$
$$-\langle n,k_\zeta,-\tfrac{1}{2}|S|l,k_\zeta,\tfrac{1}{2}\rangle\langle l,k_\zeta,\tfrac{1}{2}|k_\xi|n,k_\zeta,\tfrac{1}{2}\rangle)\ , \tag{44}$$

with

$$\langle n+1,k_\zeta,-\tfrac{1}{2}|S|n,k_\zeta,\tfrac{1}{2}\rangle=\frac{i}{\hbar(\omega_c+\omega_s)}\langle n+1,k_\zeta,-\tfrac{1}{2}|(H_A+H_C)|n,k_\zeta,\tfrac{1}{2}\rangle$$
$$=\frac{-4\sqrt{2}\sqrt{n+1}}{(\omega_c+\omega_s)R_0}\left[\frac{\delta_0}{\hbar R_0^2}(n+1-2k_\zeta^2R_0^2)F_0^*+\frac{\mu_B B_0 k_\zeta}{\hbar}\left[\frac{g''}{2}+\gamma_0\sum_i R_{i\zeta}^2R_{i+}R_{i-}\right]\right]\ , \tag{45}$$

and

$$\langle n-1,k_\zeta,-\tfrac{1}{2}|S|n,k_\zeta,\tfrac{1}{2}\rangle=\frac{-4\sqrt{2}\sqrt{n}}{(\omega_c-\omega_s)R_0}\left[\frac{\delta_0}{\hbar R_0^2}(n-2k_\zeta^2R_0^2)F_2^*+\frac{\mu_B B_0 k_\zeta}{\hbar}\gamma_0\sum_i R_{i\zeta}^2R_{i-}^2\right]\ . \tag{46}$$

Therefore,

$$\langle n,k_\zeta,-\tfrac{1}{2}|i[V,S]|n,k_\zeta,\tfrac{1}{2}\rangle\simeq\frac{-4\hbar}{m^*R_0^2}\left\{\frac{1}{\omega_c+\omega_s}\left[\frac{\delta_0F_0^*}{\hbar R_0^2}(2n+1-2k_\zeta^2R_0^2)+\frac{\mu_B B_0k_\zeta}{\hbar}\left[\tfrac{1}{2}g''+\gamma_0\sum_i R_{i\zeta}^2R_{i+}R_{i-}\right]\right]\right.$$
$$\left.+\frac{1}{\omega_c-\omega_s}\left[\frac{\delta_0F_2^*}{\hbar R_0^2}(2n+1-2k_\zeta^2R_0^2)+\frac{\mu_B B_0k_\zeta}{\hbar}\gamma_0\sum_i R_{i\zeta}^2R_{i-}^2\right]\right\}\ . \tag{47}$$

Finally, the magnetic dipole amplitude is

$$-\frac{i\hbar\omega}{4mc}\sqrt{\epsilon}\langle n,k_\zeta|\hat{\zeta}\cdot\underset{\sim}{g}\cdot(\hat{\xi}+i\hat{\eta})|n,k_\zeta\rangle=-i\frac{\hbar\omega}{4mc}\sqrt{\epsilon}4\gamma_0\left\langle n,k_\zeta\left|\sum_{\lambda,\mu}k_\lambda k_\mu\sum_i R_{i\lambda}R_{i\mu}R_{i\zeta}R_{i-}\right|n,k_\zeta\right\rangle$$
$$=-i\frac{\hbar\omega}{4mc}\sqrt{\epsilon}4\gamma_0\left[\frac{2(2n+1)}{R_0^2}\sum_i R_{i-}^2R_{i+}R_{i\zeta}+k_\zeta^2\sum_i R_{i\zeta}^3R_{i-}\right]$$
$$\equiv-\frac{i\hbar\omega}{4mc}\sqrt{\epsilon}g_{\rm EV}(n,k_\zeta)\ . \tag{48}$$

Hence, in the EV configuration, we obtain

$$M_{\nu'\nu}\simeq\langle n,k_\zeta,-\tfrac{1}{2}|(V+i[V,S])|n,k_\zeta,+\tfrac{1}{2}\rangle$$
$$\simeq\frac{4\delta_0}{\hbar R_0^2}(F_0^*+F_2^*)(2n+1-2k_\zeta^2R_0^2)+\frac{2g''\mu_B B_0}{\hbar}k_\zeta+\frac{4\gamma_0\mu_B B_0}{\hbar}k_\zeta\sum_i R_{i\zeta}^2R_{i-}(R_{i+}+R_{i-})$$
$$-4\left\{\frac{1}{1+\omega_s/\omega_c}\left[\frac{\delta_0F_0^*}{\hbar R_0^2}(2n+1-2k_\zeta^2R_0^2)+\frac{\mu_B B_0k_\zeta}{\hbar}\left[\tfrac{1}{2}g''+\gamma_0\sum_i R_{i\zeta}^2R_{i+}R_{i-}\right]\right]\right.$$
$$\left.+\frac{1}{1-\omega_s/\omega_c}\left[\frac{\delta_0F_2^*}{\hbar R_0^2}(2n+1-2k_\zeta^2R_0^2)+\frac{\mu_B B_0k_\zeta}{\hbar}\gamma_0\sum_i R_{i\zeta}^2R_{i-}^2\right]\right\}-\frac{i\hbar\omega}{4mc}\sqrt{\epsilon}g_{\rm EV}(n,k_\zeta)\ . \tag{49}$$

In the Faraday configurations $(F_\pm)\hat{\mathbf{n}}=\hat{\zeta}$, we must keep the spatial dependence of the incident radiation field $e^{iq\zeta}$ and consider as initial and final states $|n,k_\zeta,\frac{1}{2}\rangle$ and $|n,k_\zeta+q,-\frac{1}{2}\rangle$, respectively. In the $F_\pm$ configurations $\hat{\varepsilon}=(1/\sqrt{2})(\hat{\xi}\pm i\hat{\eta})$ and

$$V=\frac{1}{2\sqrt{2}}\{v_\pm, e^{iq\zeta}\}\pm\frac{\hbar\omega}{8\sqrt{2}mc}\sqrt{\epsilon}\{(\hat{\xi}\pm i\hat{\eta})\cdot \underset{\sim}{g}\cdot\sigma, e^{iq\zeta}\}\equiv V_\pm \; . \tag{50}$$

We have to calculate

$$M^{\pm}_{\bar{\nu}\nu}\cong\langle n,k_\zeta+q,-\tfrac{1}{2}|(V_\pm+i[V_\pm,S])|n,k_\zeta,\tfrac{1}{2}\rangle \; . \tag{51}$$

Now,

$$\begin{aligned}\langle n,k_\zeta+q,-\tfrac{1}{2}|V_\pm|n,k_\zeta,\tfrac{1}{2}\rangle &= \frac{1}{2\sqrt{2}}\langle n,k_\zeta+q,-\tfrac{1}{2}|v_\pm|n,k_\zeta+q,\tfrac{1}{2}\rangle+\frac{1}{2\sqrt{2}}\langle n,k_\zeta,-\tfrac{1}{2}|v_\pm|n,k_\zeta,\tfrac{1}{2}\rangle\\ &\quad\pm\frac{\hbar\omega\sqrt{\epsilon}}{8\sqrt{2}mc}\langle n,k_\zeta+q|(\hat{\xi}\pm i\hat{\eta})\cdot\underset{\sim}{g}\cdot(\hat{\xi}+i\hat{\eta})|n,k_\zeta+q\rangle\\ &\quad\pm\frac{\hbar\omega\sqrt{\epsilon}}{8\sqrt{2}mc}\langle n,k_\zeta|(\hat{\xi}\pm i\hat{\eta})\cdot\underset{\sim}{g}\cdot(\hat{\xi}+i\hat{\eta})|n,k_\zeta\rangle \; .\end{aligned} \tag{52}$$

For the velocity matrix elements, we have

$$\begin{aligned}\langle n,k_\zeta,-\tfrac{1}{2}|v_\pm|n,k_\zeta,\tfrac{1}{2}\rangle &= \langle n,k_\zeta,-\tfrac{1}{2}|v_{0\pm}+v_{A\pm}+v_{C\pm}|n,k_\zeta,\tfrac{1}{2}\rangle\\ &=\frac{2}{\hbar}\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{\partial H_A}{\partial k_\mp}+\frac{\partial H_C}{\partial k_\mp}\right|n,k_\zeta,\frac{1}{2}\right\rangle ,\end{aligned} \tag{53}$$

where

$$\frac{2}{\hbar}\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{\partial H_A}{\partial k_-}\right|n,k_\zeta,\frac{1}{2}\right\rangle=\frac{8\delta_0}{\hbar R_0^2}(2n+1-2k_\zeta^2R_0^2)F_2^* \; , \tag{54}$$

$$\frac{2}{\hbar}\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{\partial H_A}{\partial k_+}\right|n,k_\zeta,\frac{1}{2}\right\rangle=\frac{8\delta_0}{\hbar R_0^2}(2n+1-2k_\zeta^2R_0^2)F_0^* \; , \tag{55}$$

$$\frac{2}{\hbar}\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{\partial H_C}{\partial k_-}\right|n,k_\zeta,\frac{1}{2}\right\rangle=\frac{8\gamma_0\mu_B B_0}{\hbar}k_\zeta\sum_i R_{i-}^2R_{i\zeta}^2 \; , \tag{56}$$

and

$$\frac{2}{\hbar}\left\langle n,k_\zeta,-\frac{1}{2}\left|\frac{\partial H_C}{\partial k_+}\right|n,k_\zeta,\frac{1}{2}\right\rangle=\frac{4g''\mu_B B_0}{\hbar}k_\zeta+\frac{8\gamma_0\mu_B B_0}{\hbar}k_\zeta\sum_i R_{i+}R_{i-}R_{i\zeta}^2 \; . \tag{57}$$

For the magnetic dipole contributions, we set

$$g_{F_+}(n,k_\zeta)\equiv\tfrac{1}{2}\langle n,k_\zeta|(\hat{\xi}+i\hat{\eta})\cdot\underset{\sim}{g}\cdot(\hat{\xi}+i\hat{\eta})|n,k_\zeta\rangle=4\gamma_0\left[\frac{2(2n+1)}{R_0^2}\sum_i R_{i-}^3R_{i+}+k_\zeta^2\sum_i R_{i-}^2R_{i\zeta}^2\right] , \tag{58}$$

and

$$\begin{aligned}g_{F_-}(n,k_\zeta)&\equiv\tfrac{1}{2}\langle n,k_\zeta|(\hat{\xi}-i\hat{\eta})\cdot\underset{\sim}{g}\cdot(\hat{\xi}+i\hat{\eta})|n,k_\zeta\rangle\\ &=g_0+2g'\left[k_\zeta^2+\frac{2n+1}{R_0^2}\right]+2g''\frac{2n+1}{R_0^2}+4\gamma_0\left[\frac{2(2n+1)}{R_0^2}\sum_i R_{i-}^2R_{i+}^2+k_\zeta^2\sum_i R_{i+}R_{i-}R_{i\zeta}^2\right] .\end{aligned} \tag{59}$$

For the terms involving S, we get, to first order,

$$\begin{aligned}\langle n,k_\zeta+q,-\tfrac{1}{2}|i[V_\pm,S]|n,k_\zeta,\tfrac{1}{2}\rangle&\simeq\left\langle n,k_\zeta+q,-\frac{1}{2}\left|i\left[\frac{1}{2\sqrt{2}}\{v_{0\pm},e^{iq\zeta}\},S\right]\right|n,k_\zeta,\frac{1}{2}\right\rangle\\ &=\frac{i\hbar}{m^*\sqrt{2}}\langle n,k_\zeta+q,-\tfrac{1}{2}|[e^{iq\zeta}k_\pm,S]|n,k_\zeta,\tfrac{1}{2}\rangle\\ &=\frac{i\hbar}{m^*\sqrt{2}}\sum_{m=n\pm1}(\langle n,k_\zeta|k_\pm|m,k_\zeta\rangle\langle m,k_\zeta,-\tfrac{1}{2}|S|n,k_\zeta,\tfrac{1}{2}\rangle\\ &\qquad-\langle n,k_\zeta+q,-\tfrac{1}{2}|S|m,k_\zeta+q,\tfrac{1}{2}\rangle\langle m,k_\zeta+q|k_\pm|n,k_\zeta+q\rangle) \; .\end{aligned} \tag{60}$$

Finally, combining Eqs. (45), (46), and (50)–(60), for the F_+ configuration, we obtain

$$\langle n,k_\xi+q,-\tfrac{1}{2}|(V_+ +i[V_+,S])|n,k_\xi,\tfrac{1}{2}\rangle=\frac{4\sqrt{2}\delta_0F_2^*}{\hbar R_0^2}\left[2n+1-[(k_\xi+q)^2+k_\xi^2]R_0^2 -\frac{1}{1-\omega_s/\omega_c}[2n+1-2(n+1)(k_\xi+q)^2R_0^2+2nk_\xi^2R_0^2]\right] +\frac{4\sqrt{2}\gamma_0\mu_B B_0}{\hbar}\left[\sum_i R_{i\xi}^2R_{i-}^2\right]\left[k_\xi+\frac{q}{2}-\frac{1}{1-\omega_s/\omega_c}[k_\xi+(n+1)q]\right] +\frac{\hbar\omega\sqrt{\epsilon}}{4\sqrt{2}mc}[g_{F_+}(n,k_\xi+q)+g_{F_+}(n,k_\xi)]\,, \tag{61}$$

while the corresponding result for the F_- configuration is

$$\langle n,k_\xi+q,-\tfrac{1}{2}|(V_- +i[V_-,S])|n,k_\xi,\tfrac{1}{2}\rangle$$
$$=\frac{4\sqrt{2}\delta_0F_0^*}{\hbar R_0^2}\left[2n+1-(k_\xi+q)^2R_0^2-k_\xi^2R_0^2-\frac{1}{1+\omega_s/\omega_c}[2n+1-2(n+1)k_\xi^2R_0^2+2n(k_\xi+q)^2R_0^2]\right] +\frac{4\sqrt{2}\mu_B B_0}{\hbar}\left[\tfrac{1}{2}g''+\gamma_0\sum_i R_{i\xi}^2R_{i+}R_{i-}\right]\left[k_\xi+\frac{q}{2}-\frac{1}{1+\omega_s/\omega_c}(k_\xi-nq)\right]-\frac{\hbar\omega\sqrt{\epsilon}}{4\sqrt{2}mc}[g_{F_-}(n,k_\xi+q)+g_{F_-}(n,k_\xi)]\,. \tag{62}$$

III. MIXING OF CONDUCTION- AND VALENCE-BAND WAVE FUNCTIONS AND ELECTRON-SPIN RESONANCE

In the effective-mass formalism, we focus on a limited number of states and, correspondingly, construct a projected Hamiltonian $\hat{H}_{\text{eff}}$ by means of Löwdin[13] perturbation theory. Then, in order to calculate the velocity matrix elements between states belonging to the chosen subspace, we just take the elements of $(i/\hbar)[\hat{H}_{\text{eff}},\mathbf{r}]$. While this scheme can give energy eigenvalues as accurate as we want, it fails to give some of the corrections to the velocity matrix elements due to the admixture of the chosen states with other bands. From a formal point of view, this happens because the velocity associated with the projected Hamiltonian does not reproduce exactly the corresponding projection of the velocity associated with the total Hamiltonian. Physically, the problem arises because the eigenstates do have a "tail" outside the chosen subspace. From a group-theoretical viewpoint, it is, of course, possible to get a projected invariant expansion of the velocity that would contain all possible contributions, but this expansion does not coincide, in general, with the velocity associated with the projected invariant expansion of the Hamiltonian. In the following, a simple model for InSb is worked out to elucidate this difficulty. The conclusion will be that, due to the admixture of hole wave functions into the "conduction-electron" eigenstates, an additional contribution to the spin-resonance amplitude is present; this term is inversely proportional to the band gap and cannot be obtained using a 2×2 effective Hamiltonian to describe the electronic states.

We assume that the Γ_6, Γ_7, and Γ_8 bands of InSb do not at all mix with other bands and that their mutual interaction is described by the following 8×8 Hamiltonian:

$$\hat{H}=\begin{bmatrix} O & \hat{C} \\ \hat{C}^\dagger & \hat{B}\end{bmatrix} \begin{matrix}\text{conduction band (CB)}\,, \\ \text{valence band (VB)}\,,\end{matrix} \tag{63}$$

$$\hat{B}=\begin{bmatrix} -E_g 1_{4\times4} & O \\ O & (-E_g-\Delta)1_{2\times2}\end{bmatrix}, \tag{64}$$

$$\hat{C}=P\begin{bmatrix} \frac{1}{\sqrt{2}}k_+ & -\sqrt{2/3}k_z & -\frac{1}{\sqrt{6}}k_- & 0 & \frac{1}{\sqrt{3}}k_z & \frac{1}{\sqrt{3}}k_- \\ 0 & \frac{1}{\sqrt{6}}k_+ & -\sqrt{2/3}k_z & -\frac{1}{\sqrt{2}}k_- & \frac{1}{\sqrt{3}}k_+ & -\frac{1}{\sqrt{3}}k_z \end{bmatrix}, \tag{65}$$

where E_g is the energy gap, Δ the spin-orbit splitting between Γ_7 and Γ_8 bands, and P the Kane momentum matrix element between conduction and valence states.[14] The symbols O represent matrices all whose elements are zero.

In this model, $\hat{H}$ is the total exact Hamiltonian, but we are only interested in the conduction-band subspace. To obtain the 2×2 projected Hamiltonian, we write the exact eigenstates $|\psi\rangle$ as $(|\psi^c\rangle+|\psi^v\rangle)$, where $|\psi^c\rangle$ and $|\psi^v\rangle$ have only components in the conduction and valence bands, respectively; then, $\hat{H}|\psi\rangle=E|\psi\rangle$ gives

$$\hat{C}|\psi^v\rangle=E|\psi^c\rangle \tag{66}$$

and

$$\hat{C}^\dagger|\psi^c\rangle+\hat{B}|\psi^v\rangle=E|\psi^v\rangle . \tag{67}$$

Inverting the second equation, we have

$$|\psi^v\rangle=\frac{1}{E-\hat{B}}\hat{C}^\dagger|\psi^c\rangle , \tag{68}$$

which, substituted into the first, gives

$$\hat{C}\frac{1}{E-\hat{B}}\hat{C}^\dagger|\psi^c\rangle=E|\psi^c\rangle . \tag{69}$$

We define the operator

$$\hat{H}_{\text{eff}}=\hat{C}\frac{1}{E-\hat{B}}\hat{C}^\dagger ;$$

$\hat{H}_{\text{eff}}$ depends on its eigenvalue E and $\hat{H}_{\text{eff}}(E)|\psi^c\rangle=E|\psi^c\rangle$ must be solved self-consistently. The expression for $\hat{H}_{\text{eff}}(E)$ can be cast in the following form:[3]

$$\hat{H}_{\text{eff}}(E)=\frac{\hbar^2k^2}{2m^*(E)}+\tfrac{1}{2}g(E)\mu_B\boldsymbol{\sigma}\cdot\mathbf{B}_0 , \tag{70}$$

with

$$\frac{\hbar^2}{m^*(E)}=\tfrac{2}{3}P^2\left[\frac{2}{E+E_g}+\frac{1}{E+E_g+\Delta}\right] . \tag{71}$$

$$g(E)=\left[\frac{m}{\hbar^2}\right]\tfrac{4}{3}P^2\left[\frac{1}{E+E_g+\Delta}-\frac{1}{E+E_g}\right] . \tag{72}$$

Expanding $m^*(E)$ and $g(E)$, we get

$$\hat{H}_{\text{eff}}(E)\approx\hat{H}^0_{\text{eff}}+\hat{H}^1_{\text{eff}} , \tag{73}$$

where

$$\hat{H}^0_{\text{eff}}=\hat{H}_{\text{eff}}(E=0) , \tag{74}$$

and

$$\hat{H}^1_{\text{eff}}=\epsilon_0k^4+g'\mu_B\boldsymbol{\sigma}\cdot\mathbf{B}_0k^2+\beta_0\mu_B^2B_0^2 . \tag{75}$$

Comparing with Ogg's expansion, we have $\delta_0=\alpha_0=g''=\gamma_0\equiv0$. This is due to the very simple form of the original Hamiltonian $\hat{H}$. We note, in particular, that no inversion-symmetry–breaking term is included in this model that, thus, could also apply to a diamondlike material. Using $\hat{H}^0_{\text{eff}}+\hat{H}^1_{\text{eff}}$, we can find good approximations to the eigenvalues corresponding to the conduction band as well as good approximations to the eigenstates projected into the conduction band (i.e., $|\psi^c\rangle$).

We look now for an electric dipole contribution to the spin-flip–transition amplitude. In the 2×2 scheme, i.e., calculating matrix elements of $(i/\hbar)[(\hat{H}^0_{\text{eff}}+\hat{H}^1_{\text{eff}},\mathbf{r}]$, we do not get any contribution, even allowing for $k_\zeta\neq0$ terms. Using, instead, the velocity associated with the full 8×8 Hamiltonian $\hat{H}$, we have

$$\mathbf{v}=\frac{i}{\hbar}[\hat{H},\mathbf{r}]=\frac{i}{\hbar}\begin{bmatrix} O & [\hat{C},\mathbf{r}] \\ [\hat{C}^\dagger,\mathbf{r}] & O\end{bmatrix} \tag{76}$$

and

$$\begin{aligned}\langle\psi_f|\mathbf{v}|\psi_i\rangle&=(\langle\psi_f^c|+\langle\psi_f^v|)\mathbf{v}(|\psi_i^c\rangle+|\psi_i^v\rangle)\\
&=\frac{i}{\hbar}(\langle\psi_f^c|[\hat{C},\mathbf{r}]|\psi_i^v\rangle+\langle\psi_f^v|[\hat{C}^\dagger,\mathbf{r}]|\psi_i^c\rangle)\\
&=\frac{i}{\hbar}\left[\left\langle\psi_f^c\left|[\hat{C},\mathbf{r}]\frac{1}{E_i-\hat{B}}\hat{C}^\dagger\right|\psi_i^c\right\rangle+\left\langle\psi_f^c\left|\hat{C}\frac{1}{E_f-\hat{B}}[\hat{C}^\dagger,\mathbf{r}]\right|\psi_i^c\right\rangle\right]\\
&=\frac{i}{\hbar}\left[\left\langle\psi_f^c\left|\left[\hat{C}\frac{1}{E_f-\hat{B}}\hat{C}^\dagger\mathbf{r}-\mathbf{r}\hat{C}\frac{1}{E_i-\hat{B}}\hat{C}^\dagger\right]\right|\psi_i^c\right\rangle+\left\langle\psi_f^c\left|\left[\hat{C}\frac{\mathbf{r}}{E_i-\hat{B}}\hat{C}^\dagger-\hat{C}\frac{\mathbf{r}}{E_f-\hat{B}}\hat{C}^\dagger\right]\right|\psi_i^c\right\rangle\right] .\end{aligned} \tag{77}$$

The first term is simply

$$\langle\psi_f^c|(i/\hbar)[\hat{H}_{\text{eff}}(E),\mathbf{r}]|\psi_i^c\rangle ,$$

i.e., the velocity associated with the projected Hamiltonian; the other term [which vanishes if $E_i,E_f\ll E_g,(E_g+\Delta)$] is an extra contribution which does not appear in the usual 2×2 approach. The latter term is responsible for a $k_\zeta\neq0$ electric dipole isotropic spin-flip amplitude. In fact, a straightforward calculation gives

$$\begin{aligned}\hat{C}\frac{\mathbf{r}}{E-\hat{B}}\hat{C}^\dagger=&\tfrac{1}{3}P^2\left[\frac{2}{E+E_g}+\frac{1}{E+E_g+\Delta}\right](k_x\mathbf{r}k_x+k_y\mathbf{r}k_y+k_z\mathbf{r}k_z)\\
&+\frac{i}{3}P^2\left[\frac{1}{E+E_g+\Delta}-\frac{1}{E+E_g}\right][\sigma_x(k_y\mathbf{r}k_z-k_z\mathbf{r}k_y)+\text{c.p.}] ,\end{aligned} \tag{78}$$

and, setting $r_3=\zeta$, $r_1=(1/\sqrt{2})(\xi+i\eta)$, and $r_2=(1/\sqrt{2})(\xi-i\eta)$, we have[9,15]

$$\frac{i}{\hbar}\left\langle\psi_f^c\left|\left[\hat{C}\frac{r_\alpha}{E_i-\hat{B}}\hat{C}^\dagger-\hat{C}\frac{r_\alpha}{E_f-\hat{B}}\hat{C}^\dagger\right]\right|\psi_i^c\right\rangle\cong\frac{i}{\hbar}\left\langle l,k_\zeta,-\frac{1}{2}\left|\left[\hat{C}\frac{r_\alpha}{E_i-\hat{B}}\hat{C}^\dagger-\hat{C}\frac{r_\alpha}{E_f-\hat{B}}\hat{C}^\dagger\right]\right|j,k_\zeta,+\frac{1}{2}\right\rangle$$
$$=\left[k_\zeta\delta_{\alpha2}\delta_{jl}-i\frac{1}{R_0}\sqrt{j+1}\delta_{\alpha3}\delta_{l,i+1}\right]\Lambda\ , \tag{79}$$

with

$$\Lambda=\frac{\sqrt{2}}{3}\frac{P^2}{\hbar}\left[\frac{1}{E_g+E_f}-\frac{1}{E_g+E_i}+\frac{1}{E_g+\Delta+E_i}-\frac{1}{E_g+\Delta+E_f}\right]\simeq\frac{\sqrt{2}}{3}\frac{P^2}{\hbar}\left[\frac{1}{(E_g+\Delta)^2}-\frac{1}{E_g^2}\right]\hbar\omega_s\ . \tag{80}$$

In view of the preceding discussion, in the case of a narrow-band-gap material, the spin-resonance amplitude calculated in the preceding section is modified in the following way. For the F_- configuration [Eq. (62)], the additional term Λk_ζ is present, and for the EV configuration [Eq. (49)], the additional term is $(1/\sqrt{2})\Lambda k_\zeta$; Eqs. (61) and (39) remain unchanged. There is, therefore, no additional contribution to the spin-resonance amplitude in the OV configuration.

Finally, we mention that including in $\hat{H}_{\rm eff}$ a term like $g''\mu_B\{\sigma\cdot\mathbf{k},\mathbf{B}_0\cdot\mathbf{k}\}$ would lead to an electric dipole spin-flip amplitude of a similar structure as that above, but equating the Λ term to a g'' term would be completely wrong because the Λ term does not at all correspond to a modification of the energy levels (in the present model, $g''\equiv0$). In the literature, the spin-flip amplitude given by Eq. (79) has been called nonparabolicity allowed; we stress that it is related not to complications of the dispersion relation, but to the holelike "tail" of the electron eigenstates.

IV. APPLICATIONS TO InSb AND GaAs

In order to illustrate the theoretical results described in the preceding sections, we will now discuss several numerical examples pertinent to InSb and GaAs. For these materials extensive experimental data are available, and most of the parameters relevant to the electron-spin resonance can be determined.

We consider first the g factor.[16,17,7] This is given by Eq. (31), which, for $n=0$ and $k_\zeta=0$, reduces to

$$\langle 0,0|g_{\zeta\zeta}|0,0\rangle=g_0+\frac{2g'}{R_0^2}+\frac{4\gamma_0}{R_0^2}\sum_i R_{i+}R_{i-}R_{i\zeta}^2\ . \tag{81}$$

From the magnetic field dependence, the values $g_0=-51$ and $g'=6.0\times10^{12}$ cm^2 are obtained. Fitting the observed anisotropy, one gets $\gamma_0=8.2\times10^{-13}$ cm^2. Neglecting higher Landau levels is clearly justified, since $\hbar\omega_c/k_BT\cong90$ ($\hbar\omega_s/k_BT\simeq30$) at $B_0=40$ kG and $T=4.2$ K. Here, we consider the influence of $k_\zeta\neq0$ effects on the g factor. Their importance depends on the equilibrium distribution of the electron momenta along $\mathbf{B}_0$. In particular, the relevant quantity is the average of k_ζ^2,

$$\langle k_\zeta^2\rangle=\int dk_\zeta f(k_\zeta)k_\zeta^2\ ; \tag{82}$$

$f(k_\zeta)$, the probability that the eigenstate $|0,k_\zeta,+\frac{1}{2}\rangle$ is occupied, is given by

$$f(k_\zeta)=\frac{eB_0}{4\pi^2\hbar cn_0}\left[1+\exp\left[M+\frac{\hbar^2k_\zeta^2}{2m^*k_BT}\right]\right]^{-1}\ , \tag{83}$$

with

$$M=\frac{1}{k_BT}[\tfrac{1}{2}\hbar(\omega_c-\omega_s)-\mu]\ ,$$

where it is assumed that all electrons have $n=0$ and $s=+\frac{1}{2}$; n_0 is the electron concentration and $\mu=\mu(n_0,T,B_0)$, the chemical potential. For $B_0=40$ kG, $T=4.2$ K, and $n_0=10^{15}$ cm^{-3},we obtain

$$M\simeq0.9\ , \tag{84}$$

which implies that the electrons are not degenerate. In fact, Eq. (82) gives

$$\langle k_\zeta^2\rangle\simeq1.1\frac{m^*k_BT}{\hbar^2}\ , \tag{85}$$

or

$$R_0^2\langle k_\zeta^2\rangle\simeq1.1\frac{k_BT}{\hbar\omega_c}\simeq1.2\times10^{-2}\ , \tag{86}$$

while, assuming a Boltzmann distribution, we have simply

$$\langle k_\zeta^2\rangle=\frac{m^*k_BT}{\hbar^2}\ . \tag{87}$$

Now, the correction to the g factor due to the $k_\zeta\neq0$ effects is

$$\Delta g=\langle 0,k_\zeta|g_{\zeta\zeta}|0,k_\zeta\rangle-\langle 0,0|g_{\zeta\zeta}|0,0\rangle$$
$$=2g'k_\zeta^2+4g''k_\zeta^2+2\gamma_0k_\zeta^2\sum_i R_{i\zeta}^4\ . \tag{88}$$

In view of Eq. (86), the terms proportional to g' and γ_0 are negligible compared to the corresponding ones in Eq. (81). It is estimated[17,7] that $g''\simeq-2.0\times10^5$ a.u. $\simeq-5.7\times10^{-12}$ cm^2; thus, also the term $4g''k_\zeta^2$ is a very small correction. Furthermore, the peak of the absorption line is expected to be between the $k_\zeta=0$ position and the $k_\zeta=(\langle k_\zeta^2\rangle)^{1/2}$ position, as shown in Fig. 1, and thus the determination of the g-factor parameters is even less affected than given by Eq. (86). We notice that if Ogg's estimate for g'' is used, i.e., $g''\simeq-3.5\times10^4$ a.u.

instead of -2×10^5 a.u., the main contribution to Δg in Eq. (88) becomes $2g'k_\zeta^2$, which has a positive sign; as a consequence, the absorption line would look similar to that shown in Fig. 1, but with the asymmetric tail on the higher-field side instead of the lower.

As a second example, we consider the spin-resonance intensity in the ordinary Voigt configuration.[18,19] The transition matrix element [Eq. (39)] is

$$M_{\nu'\nu}\simeq\frac{12\delta_0}{\hbar R_0^2}\left[(1-2k_\zeta^2R_0^2)F_1^*+\frac{\hbar^2\gamma_0}{6m\delta_0}k_\zeta\sum_i R_{i-}R_{i\zeta}^3\right]+\frac{i\hbar\omega_s}{4mc}\sqrt{\epsilon}g_{\mathrm{OV}}(0,k_\zeta)\ , \tag{89}$$

the contributions due to the admixture of hole states vanishing in this configuration. Taking $\hat{\mathbf{n}}\|[110]$ and as Euler angles $\alpha=7\pi/4$, $\gamma=0$, and β arbitrary, corresponding to the angle between $\mathbf{B}_0$ and the [001] axis, we get

$$F_1^*\left[\frac{7\pi}{4},\beta,0\right]=\frac{i}{16}\sin\beta(3\cos^2\beta-1)\ , \tag{90}$$

$$\sum_i R_{i-}R_{i\zeta}^3\left[\frac{7\pi}{4},\beta,0\right]=-\tfrac{1}{4}\sin\beta\cos\beta(3\cos^2\beta-1)\ , \tag{91}$$

and, as explained above, we approximate

$$g_{\mathrm{OV}}(0,k_\zeta)\simeq g_0+\frac{2g'}{R_0^2}+\frac{2g''}{R_0^2}\equiv\tilde{g}_{\mathrm{OV}} \tag{92}$$

and

$$1-2k_\zeta^2R_0^2\simeq1\ . \tag{93}$$

We obtain

$$M_{\nu'\nu}\simeq\tfrac{3}{4}i\sin\beta(3\cos^2\beta-1)\frac{\delta_0}{\hbar R_0^2}+\tfrac{1}{4}i\frac{\hbar\omega_s}{mc}\sqrt{\epsilon}\tilde{g}_{\mathrm{OV}}-\tfrac{1}{2}\sin\beta\cos\beta(3\cos^2\beta-1)\frac{\hbar k_\zeta}{mR_0^2}\gamma_0\ . \tag{94}$$

As shown below, the last term is negligible; the first two terms interfere with each other and a very good fit to the data is obtained with

$$\frac{3\delta_0}{\hbar R_0^2}\frac{mc}{\hbar\omega_s\sqrt{\epsilon}|\tilde{g}_{\mathrm{OV}}|}\simeq6.0\ , \tag{95}$$

which gives $\delta_0\simeq66$ a.u. $\simeq2.6\times10^{-22}$ eV cm^3 (if $\tilde{g}_{\mathrm{OV}}$ is calculated using Ogg's estimates for g'', one obtains $\delta_0=56$ a.u.). We note that the last term in Eq. (94) is in quadrature with the others, and thus its contribution to the intensity with respect to the δ_0 contribution is of the order of

$$\left[\frac{\hbar^2k_\zeta}{m}\frac{\gamma_0}{\delta_0}\right]^2\simeq\left[\frac{\hbar^2}{mR_0}\frac{\gamma_0}{\delta_0}\right]^2\frac{k_BT}{\hbar\omega_c}\simeq0.029\ , \tag{96}$$

which is negligible.

We consider next the cyclotron-resonance-inactive Faraday configuration (F_-). Here, we are interested in

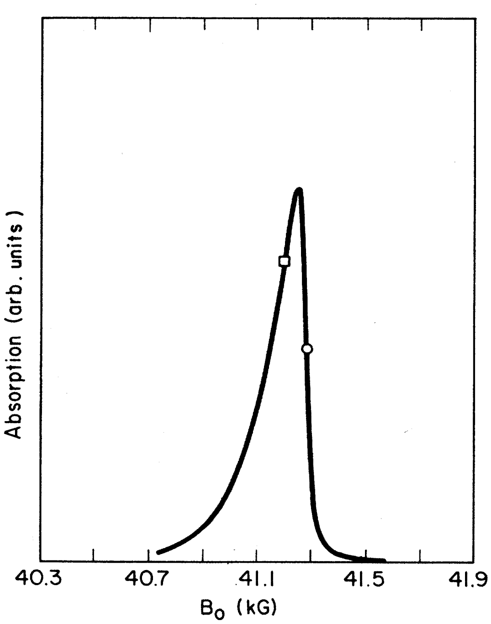

FIG. 1. Spin-resonance absorption line, the asymmetry is due to $k_\zeta\neq0$ effects [the circle corresponds to $k_\zeta=0$, while the square to $k_\zeta=(\langle k_\zeta^2\rangle)^{1/2}$].

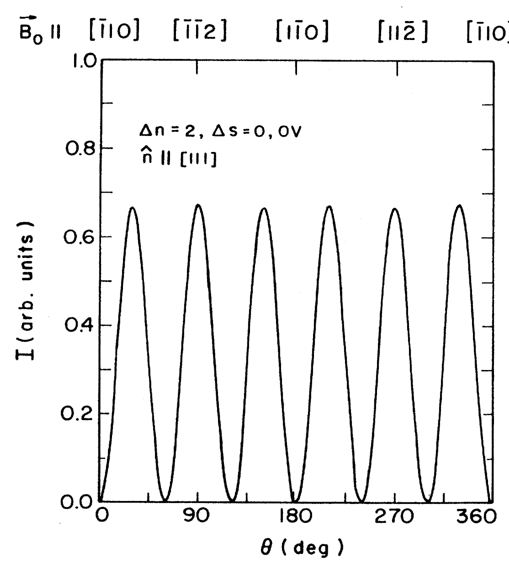

FIG. 2. Angular dependence of the intensity of $\Delta s=0$, $|\Delta n|=2$ transitions in the OV configuration with $\hat{\mathbf{n}}\|$ [111].

comparing the contribution due to the admixture of hole states as given by Eqs. (79) and (80) with all the others given by Eq. (62). In Eq. (62), we can neglect q in comparison with k_ξ; for incident wavelength $\lambda \simeq 120$ μm, for instance, we have $q = (2\pi/\lambda)\sqrt{\epsilon} \simeq 2\times 10^3$ cm^{-1}, while $(\langle k_\xi^2 \rangle)^{1/2} \simeq (1/\hbar)(m^* k_B T)^{1/2} \simeq 8\times 10^4$ cm^{-1}, at $T=4.2$ K. Then, with the same approximations described above, Eq. (62) reduces to

$$M_{\nu'\nu} = \frac{4\sqrt{2}\delta_0}{\hbar R_0^2} F_0^* \left[1 - \frac{1}{1+\omega_s/\omega_c} \right] - \frac{\hbar\omega\sqrt{\epsilon}}{2\sqrt{2}mc} \left[g_0 + \frac{2g'}{R_0^2} + \frac{2g''}{R_0^2} \right] ; \quad (97)$$

from Eqs. (79) and (80), we get the additional amplitude

$$M'_{\nu'\nu} = \Lambda k_\xi \simeq \frac{\sqrt{2}}{3} \frac{P^2}{\hbar} \left[\frac{1}{(E_g+\Delta)^2} - \frac{1}{E_g^2} \right] \hbar\omega_s k_\xi \ . \quad (98)$$

The dominant term in $M_{\nu'\nu}$ is $(4\sqrt{2}\delta_0/\hbar R_0^2)F_0^*$, which is purely imaginary and cannot interfere with $M'_{\nu'\nu}$; at $T=4.2$ K the ratio $|M'_{\nu'\nu}|^2/|M_{\nu'\nu}|^2$ is of the order of

$$\frac{\Lambda^2 \langle k_\xi^2 \rangle (\hbar R_0^2)^2}{\delta_0^2} \simeq \frac{k_B T}{\hbar\omega_c} \left[\frac{\hbar\Lambda R_0}{\delta_0} \right]^2 \simeq 0.11 \ , \quad (99)$$

$M'_{\nu'\nu}$ is therefore not completely negligible compared to $M_{\nu'\nu}$.

The term H_A in the Hamiltonian can also induce combined resonance transitions and overtones of the cyclotron resonance.[19] We take this opportunity to correct Fig. 8 of Ref. 19, which refers to parity-conserving transitions with $\Delta s = 0$ and $|\Delta n| = 2$ in the OV configuration with $\hat{n} \| [111]$.[20] The intensity for this transition is

$$\begin{aligned} I \propto |M_{\nu'\nu}|^2 &\simeq \left| \left\langle \nu' \left| \frac{1}{\hbar} \frac{\partial H_A}{\partial k_\xi} \right| \nu \right\rangle \right|^2 \\ &= \left| \frac{\delta_0}{\hbar} \left\langle n\pm 2, k_\xi \left| \frac{\partial \Omega_\xi}{\partial k_\xi} \right| \nu, k_\xi \right\rangle \right|^2 \\ &= \left| \frac{\delta_0}{\hbar} \langle n\pm 2, k_\xi | (4k_+^2 F_2 + 4k_-^2 F_2^*) | n, k_\xi \rangle \right|^2 \propto |F_2(\alpha,\beta,\gamma)|^2 \ ; \end{aligned} \quad (100)$$

this angular dependence is shown in Fig. 2.

Finally, we briefly consider GaAs. Experimental data[21,22] and theoretical estimates[23] give[3] $\delta_0 \approx 20$ eV Å^3. Experimental data[24–26] are also available for the g-factor parameters $g' \simeq 10^{-14}$ cm^2 and $\gamma_0 \approx 10^{-14}$ cm^2; we mention that from a comparison between free- and donor-bound-electron data,[24,26] it should be possible also to estimate g''.[27] We assume, as above, $n_0 = 10^{15}$ cm^{-3}, $T=4.2$ K, and $B_0 = 40$ kG; then, the electrons are not degenerate and

$$R_0^2 \langle k_\xi^2 \rangle \simeq \frac{k_B T}{\hbar\omega_c} \simeq 5\times 10^{-2} \ . \quad (101)$$

Equation (96) for GaAs gives

$$\left[\frac{\hbar^2}{mR_0} \frac{\gamma_0}{\delta_0} \right]^2 \frac{k_B T}{\hbar\omega_c} \simeq 4\times 10^{-3} \ , \quad (102)$$

while Eq. (99) yields

$$\frac{k_B T}{\hbar\omega_c} \left[\frac{\hbar\Lambda R_0}{\delta_0} \right]^2 \simeq 10^{-6} \ , \quad (103)$$

which is completely negligible.

ACKNOWLEDGMENTS

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