Energy levels of an anisotropic three-dimensional polaron in a magnetic field

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In the context of the improved Wigner-Brillouin theory, the energy levels are found of a Fröhlich polaron in a uniaxial anisotropic polar semiconductor with complex structure, placed in a magnetic field directed either along the optical axis or orthogonal to it. All sources of anisotropy that are contained in the shape of constant-energy surfaces of the bare electron, the electron–optical-phonon interaction, and the frequency spectrum of the extraordinary phonon modes are considered. Analytical results for the electron-phonon interaction correction to the Landau levels below the optical-phonon continuum are given and, numerical results for the magnetic-field dependence of the cyclotron resonance frequency at low temperature are presented for the particular case of the layered semiconductors InSe and GaSe. Although the interaction between the bare electron and quasitransverse optical-phonon modes is weak, these modes play an important role in the pinning of Landau levels. The results given by Das Sarma for a two-dimensional isotropic magnetopolaron are generalized to the anisotropic uniaxial case by taking formally $m_{\parallel}\rightarrow\infty$ in the expression of the perturbed Landau levels found when the magnetic field is directed along the optical axis, $m_{\parallel}$ being the component of the bare-electron effective-mass tensor along the optical axis.

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I. INTRODUCTION

The interaction between optical phonons and an electron moving in the presence of a magnetic field in a polar semiconductor or an ionic crystal leads to modifications of the unperturbed Landau levels, known as magnetopolaron effects. Of particular interest are the so-called resonant polaron effects[1] which characterize the magnetopolaron spectrum when the cyclotron frequency of the bare electron approaches the frequency of longitudinal-optical phonons.

Although the majority of the studies dedicated to the polaron problem deal with an isotropic system, there are some papers devoted to investigation of the polaron spectrum in anisotropic systems. Thus, theoretical methods, developed to study the polaron problem in an isotropic system have been adapted to analyze the polaron spectrum in anisotropic systems even in the presence of the external fields,[2,3] allowing the discussion of both cases, that of the piezoelectric polaron[3,4] and that of the optical polaron.[2,5]

For the particular case of small magnetic fields and taking into consideration only the anisotropy determined by the bare-electron spectrum, Hattori[2] obtained an effective Hamiltonian, similar to that of an anisotropic bare electron placed in a magnetic field, but with the components of the bare-electron mass tensor replaced by those of the polaron mass tensor. In Ref. 6 Larson analyzed the cyclotron resonance of polarons in ellipsoidal bands, a system suitable for discussion of the cyclotron resonance of holes in some cubic polar insulators with a multivalley valence band. However, the results obtained by Hattori and Larsen do not apply to the case of a uniaxial crystal with complex structure due to the presence of other sources of anisotropy that are contained in both the frequencies of the extraordinary phonon modes and the electron–optical-mode interaction. For a uniaxial crystal with complex structure, placed in a weak dc magnetic field directed along to the optical axis, the cyclotron resonance is presented[7] in the framework of intermediate-coupling theory, taking into account the contributions of all sources of anisotropy to the energy spectrum of the optical polaron.

Studies of the cyclotron resonance in the layered crystals HgI_2 (Refs. 8 and 9) and InSe (Ref. 10) deal with the anisotropic properties of the system in a simplified manner, either considering the corresponding Fröhlich Hamiltonian restricted to the one-oscillator model,[11] or introducing two anisotropic polaron coupling constants[10] $\alpha_{\perp}$ and $\alpha_{\parallel}$ for motions perpendicular and parallel, respectively, to the optical axis instead of the polaron coupling ''constants'' $\langle\alpha_{\mu}(\theta)\rangle$[12] ($\mu$ and θ denote the branch index of ''true'' optical-phonon modes and the angle between the phonon wave vector and the direction of the optical axis, the symbol $\langle\,\rangle$ meaning an angular average). In Ref. 10 the polaron coupling constants $\alpha_{\perp}$ and $\alpha_{\parallel}$, as well as the frequency of ''longitudinal'' optical phonons, seem to be merely fitting parameters rather than quantities entirely determined by the anisotropic properties of the system.

Contrary to the case of isotropic crystals where only longitudinal phonon modes interact with the electron, in a uniaxial crystal quasitransverse phonon modes also have this property. Although at weak magnetic fields the contribution of the electron–quasitransverse-mode interaction is not significant, it becomes noteworthy in the range of magnetic fields where resonant phonon effects occur.

In this paper, the contribution of the electron-phonon interaction in a uniaxial polar semiconductor to the different Landau levels is given in the framework of second-order perturbation theory, considering all the sources of anisotropy. Both geometries relevant for cyclotron resonance experiments,[8] i.e., with the magnetic field parallel or perpendicular to the optical axis, are considered. In order to avoid the real phonon emission phenomenon, the discussion is restricted to the domain of energy below the quasitransverse phonon continuum.

II. HAMILTONIAN AND ENERGY CORRECTIONS

In the effective-mass approximation the constant-energy surfaces of a conduction electron moving in a uniaxial polar

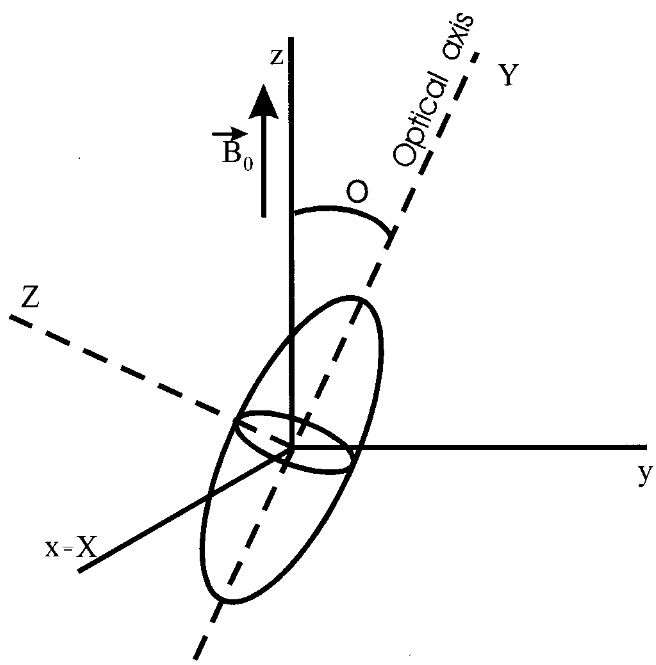

FIG. 1. The relative position of a constant-energy surface of the bare electron and the magnetic field.

semiconductor are ellipsoids of revolution having their axes coincident with the optical axis. In the presence of a dc magnetic field $\mathbf{B}_0$ making an angle Θ with the optical axis, as in Fig. 1, the Hamiltonian of the bare electron written in the symmetrical Coulomb gauge is

$$H_e=\frac{1}{2m_\perp}\left(p_x-\frac{e}{2}B_0y\right)^2+\frac{1}{2m_\perp}\left[p_z\sin\Theta-\left(p_y+\frac{e}{2}B_0x\right)\cos\Theta\right]^2+\frac{1}{2m_\parallel}\left[p_z\cos\Theta+\left(p_y+\frac{e}{2}B_0x\right)\sin\Theta\right]^2, \quad (1)$$

where x, y, z are the coordinates, p_x,p_y,p_z the components of the electron momentum, and $m_\perp,m_\parallel$ the components of the diagonal effective-mass tensor, the symbols $\perp$ and $\parallel$ corresponding to a direction that is either orthogonal or parallel to the optical axis.

In order to discuss the magnetopolaron problem we shall consider the interaction of the conduction electron with the optical phonons in an anisotropic (uniaxial) polar semiconductor so that the Hamiltonian of the system of interest has the form

$$H=H_e+H_{e\text{-ph}}+H_{\text{ph}}=H_e+\sum_{\mathbf{q},\mu}\left(\frac{V_\mu(\mathbf{q})}{\sqrt{V}}b_{\mathbf{q},\mu}e^{i\mathbf{q}\cdot\mathbf{r}}+\text{H.c.}\right)+\sum_{\mathbf{q},\mu}\hbar\omega_\mu(\mathbf{q})b^\dagger_{\mathbf{q},\mu}b_{\mathbf{q},\mu}, \quad (2)$$

where the correspondence is straightforward. In the above expression V is the volume and $b^\dagger_{\mathbf{q},\mu}$ and $b_{\mathbf{q},\mu}$ are, respectively, creation and annihilation operators for a phonon with wave vector $\mathbf{q}$, branch index μ, and frequency $\omega_\mu(\mathbf{q})$; the form of the coupling constant $V_\mu(\mathbf{q})$ was obtained by Toyozawa.[12,13]

Following Ref. 14 we perform the canonical transforms

$$p_x=g^{1/2}(\Theta)p'_x,\quad x=g^{-1/2}(\Theta)(x'+x_0), \quad (3a)$$

$$p_y=g^{-1/2}(\Theta)p'_y,\quad y=g^{1/2}(\Theta)y', \quad (3b)$$

with

$$g(\Theta)=(\cos^2\Theta+\gamma\sin^2\Theta)^{1/2},\quad \gamma=m_\perp/m_\parallel, \quad (4a)$$

$$x_0=-\frac{2(1-\gamma)}{m_\perp\omega\sqrt{g(\Theta)}}p_z\sin\Theta\cos\Theta, \quad (4b)$$

where by $\omega=eB_0g(\Theta)/m_\perp$ we have denoted the cyclotron frequency of the bare electron. This procedure reduces the form of the Hamiltonian that describes the dynamics of the bare electron in a plane orthogonal to the magnetic-field direction to that of an electron having spherical energy surfaces with an effective mass $m=m_\perp/g(\Theta)$, so that one obtains

$$H_e=\frac{1}{2m}\left[\left(p_{x'}-\frac{e}{2}B_0y'\right)^2+\left(p_{y'}+\frac{e}{2}B_0x'\right)^2\right]+\frac{p_z^2}{2m_\parallel g^2(\Theta}. \quad (5)$$

Introducing instead of the coordinates and components of the momentum the operators (A,A^+) and (B,B^+),[15]

$$A=\left(\frac{1}{2\hbar m\omega}\right)^{1/2}(p_{x'}-ip_{y'})-\frac{i}{2}\left(\frac{m\omega}{2\hbar}\right)^{1/2}(x'-iy'), \quad (6a)$$

$$B=\frac{1}{2}\left(\frac{m\omega}{2\hbar}\right)^{1/2}(x'+iy')+i\left(\frac{1}{2\hbar m\omega}\right)^{1/2}(p_{x'}+ip_{y'}) \quad (6b)$$

that satisfy the commutation relations $[A,A^+]=[B,B^+]=1$ and $[A,B]=[A,B^+]=0$, expression (5) becomes

$$H_e=\hbar\omega(A^+A+\tfrac{1}{2})+\frac{p_z^2}{2m_\parallel g^2(\Theta)}. \quad (7)$$

Having introduced the operators (A,A^+) and (B,B^+), we can now represent the Landau level as

$$|n,m,p_z\rangle=|n\rangle_A\otimes|m\rangle_B\otimes|p_z\rangle, \quad (8)$$

where $|p_z\rangle$ describes the movement of the electron along the z direction, and $(n!)^{-1/2}(A^+)^n|0\rangle_A$ and $(m!)^{-1/2}(B^+)^m|0\rangle_B$ are two independent one-dimensional harmonic oscillator states,[16] with $|0\rangle_A,|0\rangle_B$ the vacuum states of the operators A, B. However, we have to stress that here, in contradiction to the situation encountered in the case of isotropic systems, the operator $\hbar(A^+A-B^+B)$ is not the z component of the angular momentum.

Working at zero temperature with the initial unperturbed state $|n,m,p_z\rangle\otimes|0\rangle_{\rm ph}$ where $|0\rangle_{\rm ph}$ is the phonon vacuum state, the energy correction of the electron-phonon interaction to the bare-electron Landau level in the context of second-order perturbation theory is given by[17,18]

$$\Delta E_n(p_z)=\frac{1}{V}\sum_{n',q,\mu}\frac{|V_\mu(\mathbf{q})|^2}{D_{nn'}}, \tag{9}$$

where

$$D_{nn'}=(n-n')\hbar\omega+\frac{1}{2m_\parallel g^2(\Theta)}[p_z^2-(p_z-\hbar q_z)^2] -\hbar\omega_\mu(\mathbf{q})+\Delta_n, \tag{10}$$

Δ_n being determined by the actual type of perturbation theory used [$\Delta_n=0$ for the Rayleigh-Schrödinger perturbation theory (RSPT), $\Delta_n=\Delta E_n(p_z)$ for the Wigner-Brillouin perturbation theory (WBPT), and finally $\Delta_n=\Delta E_n(p_z)-\Delta E_0^{\rm RSPT}$ for the improved Wigner-Brillouin theory (WBPT)]. At low magnetic fields the Rayleigh-Schrödinger perturbation theory gives appropriate results for the magnetopolaron spectrum. Although the magnetopolaron splitting is obtained in the framework of Wigner-Brillouin perturbation theory, the calculated energy levels are not accurate, especially in the pinning region. The correct behavior of the energy levels of the excited states is obtained only for the improved Wigner-Brillouin theory.

Considering the behavior of the different Landau levels below the optical-phonon continuum and following the method described in Ref. 19, the energy shift of the nth Landau level can be put in the form

$$\Delta E_n(p_z)=-\sum_{\mathbf{q},\mu}\frac{|V_\mu(\mathbf{q})|^2}{\hbar V}\times\int_0^\infty d\tau\, e^{-[\omega_\mu(\mathbf{q})-\Delta_n/\hbar]\tau}\langle n,m,p_z|\times e^{i\mathbf{q}\cdot\mathbf{r}(\tau)}e^{-i\mathbf{q}\cdot\mathbf{r}(0)}|n,m,p_z\rangle, \tag{11}$$

where

$$\mathbf{r}(\tau)=e^{H_e\tau/\hbar}\mathbf{r}e^{-H_e\tau/\hbar}. \tag{12}$$

Using the canonical transform (3) and the expressions (6), the argument $\mathbf{q}\cdot\mathbf{r}$ of the exponential appearing in $H_{e\text{-ph}}$ can be written in terms of x_0, appropriate combinations of the phonon wave-vector components, and the operators A, A^+, B, and B^+.

The evaluation of the effect of the matrix element that appears in Eq. (11) on the electron state $|n,m,p_z\rangle$ is straightforward, so that one obtains for the energy shift (independent of m) the expression

$$\Delta E_n(p_n)=-\frac{1}{\hbar V}\sum_{\mathbf{q},\mu}|V_\mu(\mathbf{q})|^2\int_0^\infty d\tau\exp\left\{-\left[\omega_\nu(\mathbf{q})-\Delta_n/\hbar+\frac{\hbar q_z^2}{2m_\parallel g^2(\Theta)}-\frac{q_zp_z}{m_\parallel g^2(\Theta)}\right]\tau\right\}\times\exp\left[-\frac{\hbar Q^2}{2m\omega g(\Theta)}(1-e^{\omega\tau})\right]\times\sum_{p=0}^{n}\frac{c_n^p}{p!}\left[\frac{2\hbar Q^2}{m\omega g(\Theta)}\sinh^2\frac{\omega\tau}{2}\right]^p \tag{13}$$

with

$$Q^2=q_x^2+g^2(\Theta)q_y^2. \tag{14}$$

This expression will be discussed in the following in the context of the particular geometry considered, and will allow us to obtain some explicit analytical results in limiting cases.

A. Magnetic field parallel to the optical axis

In this geometry $g=1$, $\omega=eB_0/m_\perp$, and, limiting ourselves to the case of an electron with low values of p_z, $\{p_z\ll[2\hbar m_\parallel\omega_\mu(\theta)]^{1/2}\}$, where θ is the angle between the phonon wave vector and the direction of the optical axis, expression (13) reduces to

$$\Delta E_n/\hbar=-\frac{1}{2\sqrt{\pi}}\sum_\mu\int_0^\pi d\theta\sin\theta\,\omega_\mu(\theta)\times\left(\frac{\omega_\mu(\theta)}{\omega}\right)^{1/2}S^{1/2}(\theta)\alpha_\mu(\theta)\times\int_0^\infty\frac{d\tau}{\sqrt{\tau}}e^{-\{[\omega_\mu(\theta)-\Delta_n/\hbar]/\omega\}\tau}G_n(\tau,\theta), \tag{15}$$

where

$$G_n(\tau,\theta)=\sum_{p=0}^{n}C_n^p\frac{(2p-1)!!}{p!}\times\left[\frac{2\sin^2\theta}{\gamma\tau P(\tau,\theta)}\sinh^2\left(\frac{\tau}{2}\right)\right]^p\frac{1}{\sqrt{P(\tau,\theta)}}\times\left\{1+(2p+1)\frac{p_z^2\cos^2\theta}{2m_\parallel\hbar\omega}\frac{\tau}{P(\tau,\theta)}\right\}, \tag{16}$$

with

$$P(\tau,\theta)=\cos^2\theta+\frac{1-e^{-\tau}}{\gamma\tau}\sin^2\theta, \tag{17a}$$

$$s(\theta)=\cos^2\theta+\gamma^{-1}\sin^2\theta, \tag{17b}$$

the explicit expression of the polaron coupling function $\alpha_\mu(\theta)$ appropriate for this uniaxial crystal being given in Ref. 12.

In the small-magnetic-field limit $[\omega \ll \omega_\mu(\theta)]$ and in the context of RSPT, which is appropriate for this case, the expression (15) for the energy shift becomes

$$\Delta E_n/\hbar = -\sum_\mu \langle \alpha_\mu(\theta)\omega_\mu(\theta)\rangle - \frac{2n+1}{8\gamma}\omega \times \sum_\mu \left\langle \frac{\alpha_\mu(\theta)\sin^2(\theta)}{s(\theta)} \right\rangle + \frac{\omega^2}{16\gamma} \times \sum_\mu \left\langle \frac{\alpha_\mu(\theta)\sin^2\theta\cos^2\theta}{s^2(\theta)\omega_\mu(\theta)} \right\rangle - \frac{18n(n+1)+1}{128\gamma^2}\omega^2 \times \sum_\mu \left\langle \frac{\alpha_\mu(\theta)\sin^4\theta}{s^2(\theta)\omega_\mu(\theta)} \right\rangle - \frac{p_z^2}{m_\parallel \hbar}\left[\sum_\mu \left\langle \frac{\alpha_\mu(\theta)\cos^2\theta}{s(\theta)} \right\rangle + \frac{9(2n+1)}{16\gamma}\omega \sum_\mu \left\langle \frac{\alpha_\mu(\theta)\sin^2\theta\cos^2\theta}{\omega_\mu(\theta)s(\theta)} \right\rangle \right], \quad (18)$$

where the symbol $\langle\,\rangle$ means the angular average

$$\langle f(\theta)\rangle = \frac{1}{2}\int_0^\pi f(\theta)\sin\theta\, d\theta. \quad (19)$$

Taking $p_z=0$ in Eq. (18), for the particular case of an isotropic crystal with simple structure, the magnetic-field correction to the electron-phonon self-energy reduces to that presented in Ref. 19.

Defining the cyclotron resonance frequency $\Omega_C^\parallel$ (the symbol $\parallel$ referring to the direction of the magnetic field parallel to the optical axis) as the energy difference between $E_1(p_z=0)$ and $E_0(p_z=0)$, one obtains for the cyclotron mass $M_C^\parallel = eB_0/\Omega_C^\parallel$

$$\left(\frac{M_C^*}{m_\perp}\right)^{-1} = 1 - \frac{1}{4\gamma}\sum_\mu \left\langle \frac{\alpha_\mu(\theta)\sin^2\theta}{s(\theta)} \right\rangle - \frac{9\omega}{32\gamma^2}\sum_\mu \left\langle \frac{\alpha_\mu(\theta)\sin^4\theta}{s^2(\theta)\omega_\mu(\theta)} \right\rangle, \quad (20)$$

an expression that results by imposing the condition of small electron-phonon coupling in the relation (33) of Ref. 7. By considering weak electron–optical-phonon coupling in the expression (37) of Ref. 7, the expressions for both the cyclotron mass and the effective mass of the motion along the z direction reduce, in the limit $\omega \to 0$, to the forms of the components $M_\perp$ and $M_\parallel$ of the polaron effective-mass tensor:

$$M_C^* \to M_\perp = m_\perp \left[1 - \frac{1}{4\gamma}\sum_\mu \left\langle \frac{\alpha_\mu(\theta)\sin^2\theta}{s(\theta)} \right\rangle \right]^{-1}, \quad (21a)$$

$$M_\parallel = m_\parallel \left[1 - \frac{1}{2}\sum_\mu \left\langle \frac{\alpha_\mu(\theta)\cos^2\theta}{s(\theta)} \right\rangle \right]^{-1}. \quad (21b)$$

Relations (21) could also be obtained by performing the calculations in expression (6) of Ref. 5 and taking into account the anisotropy of the components of the dielectric tensor.

In the limit of large magnetic fields only a numerical solution of Eq. (15) can be found, every Landau level E_n obtained in the context of IWBPT being pinned to $\hbar\omega_{\mathrm{TO},l} + \hbar\omega/2 + \Delta E_0^{\mathrm{RSPT}}$, where by $\omega_{\mathrm{TO},l}$ we have denoted the lowest transverse-optical frequency in the phonon spectrum. As a by-product of the above calculations, the expression for the energy shift for a two-dimensional (2D) electron interacting with a 3D anisotropic phonon system is obtained by formally taking $m_\parallel \to \infty$ in Eq. (15).

In terms of a polaronic coupling function defined through the relation

$$\tilde{\alpha}_\mu(\theta) = \sin\theta \lim_{m_\parallel \to \infty} \alpha_\mu(\theta), \quad (22)$$

the 2D energy shift can be expressed as

$$\Delta E_n^{(2D)}/\hbar = -\frac{1}{2}\sum_\mu \int_0^\pi d\theta\, \tilde{\alpha}_\mu(\theta)\omega_\mu(\theta)\left(\frac{\omega_\mu(\theta)}{\omega}\right)^{1/2} \times \sum_{p=0}^n c_n^p \left[\frac{(2p-1)!!}{2^p}\right]^2 \frac{1}{p!} \times \frac{\Gamma((\omega_\mu(\theta) - \Delta_n^{(2D)}/\hbar)/\omega - p)}{\Gamma(\omega_\mu(\theta) - \Delta_n^{2D)}/\hbar/\omega + \frac{1}{2})}, \quad (23)$$

a result that generalizes the expression (15) of Ref. 19 to this anisotropic case.

In the limit of small magnetic fields and in the framework of RSPT, the 2D energy shift becomes

$$\Delta E_n^{(2D)}/\hbar = -\frac{1}{2}\sum_\mu \int_0^\pi d\theta\, \tilde{\alpha}_\mu(\theta)\omega_\mu(\theta) \times \left[1 + \frac{2n+1}{8}\left(\frac{\omega}{\omega_\mu(\theta)}\right) + \frac{18n(n+1)+1}{128}\left(\frac{\omega}{\omega_\mu(\theta)}\right)^2 + \cdots \right], \quad (24)$$

an expression that agrees for an isotropic system with that obtained by Das Sarma[20] and by Larsen.[21] For large magnetic fields, and for $n\omega \cong \omega_\mu(\theta)$ one obtains

$$\Delta E_n^{(2D)}/\hbar = -\frac{\sqrt{\omega}}{\sqrt{\pi}}\frac{(2n-1)!!}{2^{n+1}n!}\sum_\mu \int_0^\pi d\theta \times \frac{\tilde{\alpha}_\mu(\theta)[\omega_\mu(\theta)]^{3/2}}{\sqrt{\omega_\mu(\theta) - \Delta_n^{(2D)}/\hbar - n\omega}}, \quad (25)$$

leading to the same pinning level for the corresponding Landau level as in the 3D case, $\hbar\omega_{\mathrm{TO},l} + \hbar\omega/2 + \Delta E_0^{\mathrm{RSPT}}$, but with a different coupling constant.

B. Magnetic field orthogonal to the optical axis

In this geometry $g = \gamma^{1/2}$, $\omega = eB_0/(m_\perp m_\parallel)^{1/2}$, and the optical axis can be chosen as the polar axis (y axis according to Fig. 1) based on the axial symmetry of both the optical-phonon spectrum and the electron-phonon interaction. In this case the expression for the energy shift ΔE_n becomes

$$\Delta E_n(p_z)/\hbar = -\frac{\gamma^{1/2}}{2\pi^2}\sum_\mu \int_0^\pi d\theta \sin\theta\, \alpha_\mu(\theta) s^{1/2}(\theta)\omega_\mu(\theta)\left(\frac{\omega_\mu(\theta)}{\omega}\right)^{1/2}\int_0^\infty \frac{du}{\sqrt{u}} \exp\left(-\frac{\omega_\mu(\theta)-\Delta_n/\hbar}{\omega}u\right)$$
$$\times\int_0^{2\pi} d\varphi \int_0^\infty dz \exp\left[-z^2\Gamma(\theta,\varphi,u)+\left(\frac{2u}{\hbar m_\perp \omega}\right)^{1/2} z p_z \sin\theta\sin\varphi\right]\times\sum_{p=0}^{n} C_n^p \frac{1}{p!}\left[\frac{4z^2}{u}\sinh^2\left(\frac{u}{2}\right)\right.$$
$$\left.\times(\sin^2\theta\cos^2\varphi+\gamma\cos^2\theta)\right]^p, \tag{26}$$

where

$$\Gamma(\theta,\varphi,u) = \sin^2\theta\sin^2\varphi + (\sin^2\theta\cos^2\varphi+\gamma\cos^2\theta)F(u) \tag{27}$$

with

$$F(u) = (1-e^{-u})/u, \tag{28}$$

θ and φ being the polar and the azimuthal angle of the phonon wave-vector direction, respectively.

In the domain of small magnetic fields and for low values of p_z, by keeping all the terms up to second order in $[\omega/\omega_\mu(\theta)]$ and fourth order in $\{p_z/[2\hbar m_\perp \omega_\mu(\theta)]^{1/2}\}$, respectively, the above expression for the energy shift can be reduced to the form

$$\Delta E_n(p_z)/\hbar = -\sum_\mu \langle \alpha_\mu(\theta)\omega_\mu(\theta)\rangle - \left(\frac{p_z^2}{2m_\perp}\right)\frac{1}{4\hbar\gamma}\sum_\mu \left\langle\frac{\alpha_\mu(\theta)\sin^2\theta}{s(\theta)}\right\rangle - \frac{9}{64}\left(\frac{p_z^2}{2m_\perp}\right)\frac{1}{\hbar^2\gamma^2}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)\sin^4\theta}{\omega_\mu(\theta)s^2(\theta)}\right\rangle$$
$$-\frac{(2n+1)}{8}\frac{\omega}{\gamma}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)(\gamma\cos^2\theta+\frac{1}{2}\sin^2\theta)}{s(\theta)}\right\rangle + \frac{\omega^2}{16}\frac{1}{\gamma}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)(\gamma\cos^2\theta+\frac{1}{2}\sin^2\theta)}{\omega_\mu(\theta)s(\theta)}\right\rangle$$
$$-\frac{9}{32}(2n+1)\frac{p_z^2}{2m_\perp}\frac{\omega}{\hbar\gamma^2}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)(\gamma\cos^2\theta+\frac{1}{4}\sin^2\theta)\sin^2\theta}{\omega_\mu(\theta)s^2(\theta)}\right\rangle$$
$$-\frac{9}{1024}(2n^2+2n+1)\frac{\omega^2}{\gamma^2}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)(8\gamma^2\cos^4\theta+8\gamma\sin^2\theta\cos^2\theta+3\sin^4\theta)}{\omega_\mu(\theta)s^2(\theta)}\right\rangle. \tag{29}$$

From the expression of the cyclotron resonance frequency, in the limit of very small magnetic fields, denoted by $\Omega_C^\perp$ in this geometry, one obtains for the corresponding cyclotron mass $M_C^\perp$ the form

$$M_C^\perp = (m_\parallel m_\perp)^{1/2}\left[1-\frac{1}{8\gamma}\times\sum_\mu\left\langle\frac{\alpha_\mu(\theta)(2\gamma\cos^2\theta+\sin^2\theta)}{s(\theta)}\right\rangle\right]^{-1}. \tag{30}$$

In the same framework of a small electron–optical-phonon interaction, the expression (30) becomes

$$M_C^\perp = (M_\perp M_\parallel)^{1/2}, \tag{31}$$

where the components of the polaron mass tensor, $M_\perp$ and $M_\parallel$, are given by the relations (21).

Neglecting the anisotropy determined by both sources, namely, the spectrum of the optical phonons and their interaction with the conduction electron, Hattori[2] obtained in intermediate-coupling theory for an arbitrary direction of the magnetic field more general expressions than Eqs. (21a) and (31) presented in our paper.

Combining Eqs. (17b), (21a), and (30), one obtains

$$2\left[\left(1-\frac{m_\perp}{M_C^\parallel}\right)+2\left(1-\frac{\sqrt{m_\perp m_\parallel}}{M_C^\perp}\right)\right] = \sum_\mu \langle\alpha_\mu(\theta)\rangle, \tag{32}$$

which reduces, in the case of an isotropic system, to the classical result[22]

$$M_P = m/(1-\alpha/6), \tag{33}$$

where by M_P and m we have denoted the polaron mass and the bare-electron mass, respectively, α being the Fröhlich dimensionless coupling constant.

Since we are interested here in discussing the cyclotron resonance phenomenon, we shall simplify the expression (26), disregarding the p_z dependence. We evaluate the expression obtained by integration over z and φ variables in Eq. (26) for large values of the argument u,[19] in the domain of magnetic fields where resonant magnetopolaron effects are important $[n\omega \cong \omega_\mu(\theta)]$. The result is $\sqrt{\pi}e^{nu}/(n \sin\theta)$, which finally gives the energy shift,

$$\Delta E_n/\hbar = -\frac{\gamma^{1/2}}{2n\pi}\sum_\mu \int_0^\pi d\theta\, \alpha_\alpha(\theta)\omega_\mu(\theta) \times \left(\frac{s(\theta)\omega_\mu(\theta)}{\omega_\mu(\theta)-\Delta_n/\hbar - n\omega}\right)^{1/2}. \tag{34}$$

This form reduces to the expression (25) of Ref. 19 in the case of an isotropic polaron.

The integration over z and φ variables in Eq. (26) can be performed exactly for the first Landau levels so that the corresponding energy shift can be put in the form

$$\Delta E_0/\hbar = -\frac{\gamma^{1/2}}{\pi^{3/2}}\sum_\mu \int_0^\pi d\theta\, \alpha_\mu(\theta)s^{1/2}(\theta)\omega_\mu(\theta) \times \left(\frac{\omega_\mu(\theta)}{\omega}\right)^{1/2}\int_0^\infty \frac{du}{\sqrt{u}} e^{-[\omega_\mu(\theta)/\omega]u}J_0(\theta,u), \tag{35a}$$

$$\Delta E_1/\hbar = -\frac{\gamma^{1/2}}{\pi^{3/2}}\sum_\mu \int_0^\pi d\theta\, \alpha_\mu(\theta)s^{1/2}(\theta)\omega_\mu(\theta)\left(\frac{\omega_\mu(\theta)}{\omega}\right)^{1/2} \times \int_0^\infty \frac{du}{\sqrt{u}} e^{-\{[\omega_\mu(\theta)-\Delta_1/\hbar]/\omega\}u}[J_0(\theta,u)+J_1(\theta,u)], \tag{35b}$$

where

$$J_0(\theta,u) = \frac{a}{[1-F(u)]^{1/2}}K(a), \tag{36a}$$

$$J_1(\theta,u) = \frac{2a}{[1-F(u)]^{3/2}}\left(\frac{\sinh^2(u/2)}{u}\right)\left[\frac{E(a)}{F(a)} - K(a)\right], \tag{36b}$$

$$a = [1-F(u)]^{1/2}[\sin^2\theta + \gamma F(u)\cos^2\theta]^{-1/2}\sin\theta, \tag{37}$$

$K(a)$ and $E(a)$ being the complete elliptic integrals of the first and second kind, respectively.

III. NUMERICAL RESULTS AND CONCLUDING REMARKS

In the following we shall use the expressions (15) and (35) for the energy shift to obtain the magnetic-field dependence of the cyclotron resonance frequency at zero temperature, in the case of the layered materials InSe and GaSe. For both materials the appropriate form of the dielectric function can be described in the context of a two-oscillator model determined by the values of the parameters. For InSe,[23,24]

$$\varepsilon_\perp(\infty) = 7.8, \quad \omega_{TO}^\perp = 180\ \text{cm}^{-1}, \quad \omega_{LO}^\parallel = 200\ \text{cm}^{-1},$$

$$\varepsilon_\parallel(\infty) = 8.9, \quad \omega_{TO}^\parallel = 190\ \text{cm}^{-1}, \quad \omega_{LO}^\perp = 220\ \text{cm}^{-1},$$

and for GaSe,[25]

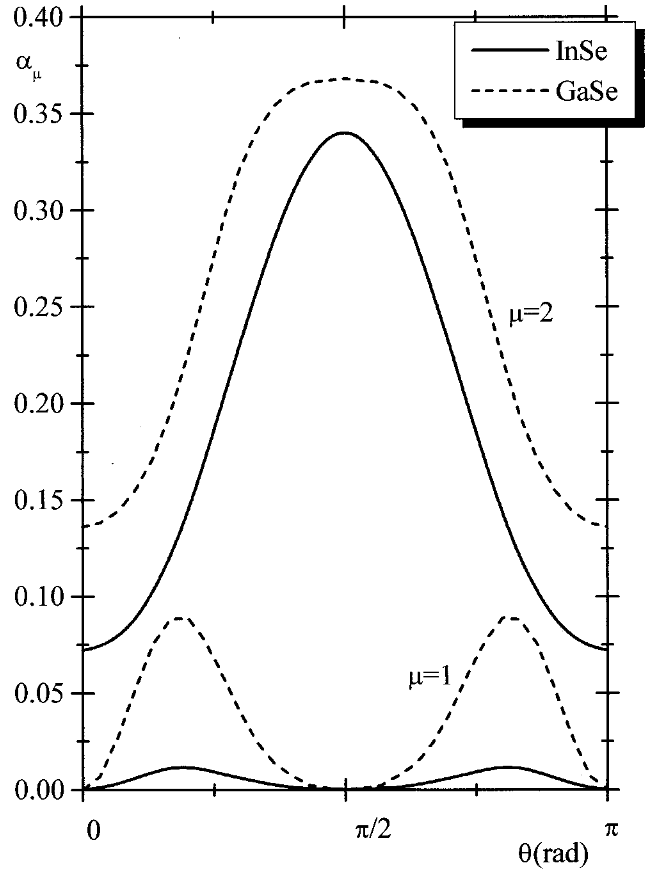

FIG. 2. The angular dependence of the polaron coupling functions $\alpha_\mu(\theta)$ for the two branches of the extraordinary phonon modes for InSe (solid curves) and GaSe (dashed curves).

$$\varepsilon_\perp(\infty) = 7.44, \quad \omega_{TO}^\perp = 213.5\ \text{cm}^{-1}, \quad \omega_{LO}^\parallel = 245.5\ \text{cm}^{-1},$$

$$\varepsilon_\parallel(\infty) = 5.76, \quad \omega_{TO}^\parallel = 237\ \text{cm}^{-1}, \quad \omega_{LO}^\perp = 254.7\ \text{cm}^{-1},$$

where $\varepsilon_\alpha(\infty)$, ω_{TO}^α, and ω_{LO}^α $(\alpha = \perp, \parallel)$ are the high-frequency dielectric constants, the frequencies of the transverse-phonon modes, and the frequencies of the longitudinal-phonon modes along the principal directions, respectively. Together with the values of the mass-tensor components of the bare electron $(m_\perp = 0.131m_0,\ m_\parallel = 0.081m_0)$ for InSe (Ref. 26) $(m_\parallel = 0.17m_0,\ m_\parallel = 0.3m_0)$ for GaSe,[27,28] the above parameters allow us to obtain the angular dependence of the polaron coupling functions $\alpha_\mu(\theta)$ for the two branches $(\mu = 1,2)$ of the phonon modes involved.

The components of the effective-mass tensor of the bare electron are generally obtained either by extracting them from cyclotron resonance measurements at low magnetic fields (Refs. 26) or by analyzing, additionally to the study of the electronic transport properties, the exciton optical properties (Ref. 27). Sometimes, a combination of the aforementioned approaches is used. Thus, for InSe, the components of the effective-mass tensor of the bare electron, obtained by a self-consistent procedure, can be considered as fitting parameters only for the results of the cyclotron resonance measurements performed at low magnetic fields. However, in the domain of high magnetic fields, which is of interest for us

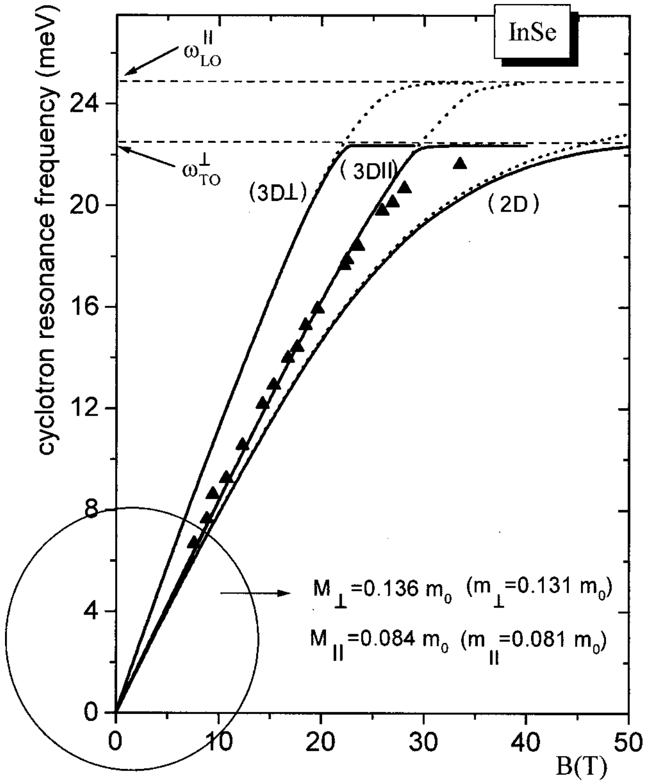

FIG. 3. The cyclotron resonance frequency vs magnetic field in InSe. The solid curves marked (3D⊥), (3D∥), and (2D), corresponding to the direction of the magnetic field orthogonal to the optical axis ⊥ or parallel to it ∥ for a 3D and to a 2D electron, respectively, are obtained (in the framework of IWBPT) by taking into account the contribution of the whole extraordinary optical-phonon spectrum. The cyclotron resonance frequency as a function of the magnetic field obtained in the mentioned geometry, and without the contribution of the quasitransverse phonon modes, is presented with dotted lines. The experimental results obtained in Ref. 10 are plotted by triangles.

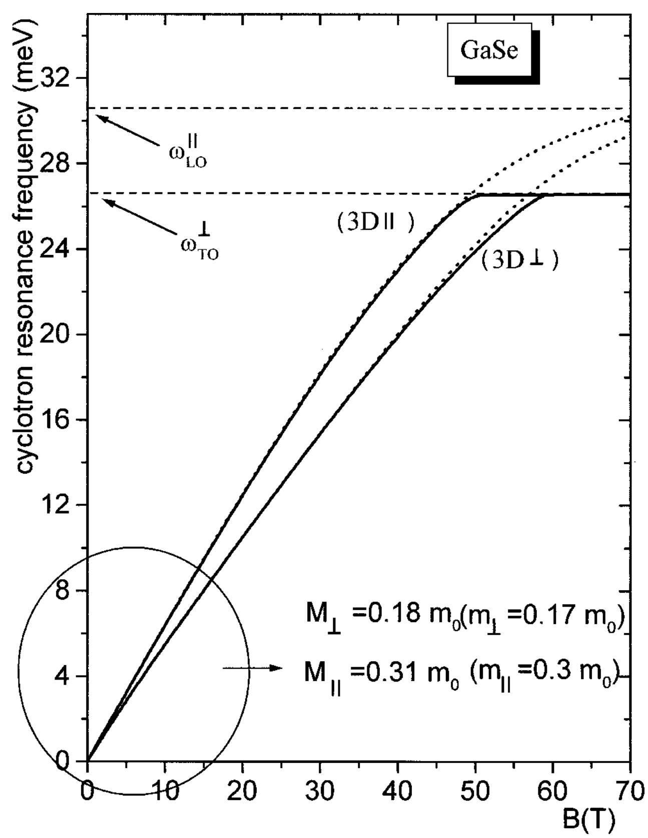

FIG. 4. The cyclotron resonance frequency vs magnetic field in GaSe. The symbols (3D⊥) and (3D∥) and the meaning of the curves are explained in the caption of Fig. 3. The curves are obtained by using the improved Wigner-Brillouin perturbation theory.

regarding the behavior of the cyclotron resonance frequency, the aforementioned quantities are not freely chosen parameters.

The polaron coupling functions corresponding to the electron–optical-phonon interaction with quasitransverse extraordinary phonon modes ($\mu=1$) and with quasilongitudinal extraordinary phonon modes ($\mu=2$) are presented in Fig. 2, with sold lines for InSe and dashed lines for GaSe. Although the polaron coupling function for quasitransverse phonon modes is small compared to that for quasilongitudinal phonon modes, the presence of the continuum frequency distribution of the quasitransverse modes in the domain $[\omega_{TO}^{\perp},\omega_{TO}^{\parallel}]$ situated at lower frequencies than the corresponding domain of quasilongitudinal phonon modes plays an important role in the cyclotron resonance phenomenon in the range of magnetic fields for which the cyclotron resonance frequency of the bare electron is in the domain of quasitransverse mode frequencies.

The cyclotron resonance frequency versus magnetic field in InSe (in the context of IWBPT) is presented in Fig. 3, the solid lines marked with the symbols (3D∥), (3D⊥), and (2D) representing, respectively, the cases of the magnetic field directed along the optical axis (∥) or orthogonal to it (⊥), for a 3D or a 2D electron interacting with all the extraordinary optical phonon modes. Customarily, the behavior of the cyclotron resonance frequency determined by Eqs. (18), (24), and (29) for the energy shift in the domain of small magnetic fields is used to obtain the components of the effective-mass tensor for the bare electron. In the case of the magnetic field orthogonal to the optical axis, expression (30) for the cyclotron mass justifies the analysis of cyclotron resonance data in the perturbational approach developed in Ref. 8. When the cyclotron resonance frequency of the bare electron is in the domain of quasitransverse mode frequencies, the curves that give the magnetic-field dependence of the cyclotron resonance frequency present an important contribution of the magnetopolaron splitting effect, and are pinned to the lowest value ($\omega_{TO}^{\perp}$) of the frequency phonon spectrum for higher values of the magnetic field. The curves of the cyclotron resonance frequency versus magnetic field in the geometries discussed above, without the contribution of the quasitransverse phonon modes, are presented with dotted lines in Fig. 3. These curves are pinned to the $\omega_{LO}^{\parallel}$ frequency.

Consistent with the theoretical method used here to obtain the energy shift for the magnetopolaron below the phonon continuum, we discuss only the lower branch of the magnetopolaron spectrum, which contributes to the experimental results obtained in Ref. 10 [see Fig. 2(a) of that reference] and is plotted by triangles in Fig. 3. Compared to our theoretical curve (3D∥), which presents the magnetic-field dependence of the cyclotron resonance frequency, we have to admit that the corresponding theoretical curve marked with the symbol (3D) in Fig. 2(a) of Ref. 10 better fits the experimental points. However, we have to stress that, contrary to the mentioned work, where the polaron coupling constants $\alpha_\perp$ and $\alpha_\parallel$ for motions perpendicular and parallel to the optical axis, as well as the frequency ω_{LO} of the ''longitudinal''-optical phonons are fitting parameters, we have no such parameters here. Of course, taking into account the quasi-two-dimensional behavior of the electron gas formed in the vicinity of stacking faults in InSe,[29] which is manifest at very low temperatures, we can improve the fit by considering a finite z extent[10] of the electron wave function. This approach, which reformulates the whole problem considered here, allowing us to choose a curve situated between the (2D) and (3D∥) curves of Fig. 3, by considering the finite z extent of the electron wave function as a fitting parameter and which realizes the best fitting of the experimental points, will be discussed in the future.

Similar results obtained for the magnetic-field dependence of the cyclotron resonance in GaSe are presented in Fig. 4. Because $\gamma_{\mathrm{InSe}}>1$ and $\gamma_{\mathrm{GaSe}}<1$ the curves (3D∥) and (3D⊥) in GaSe are in the reverse order compared with the same curves obtained in InSe.

In the framework of the IWBT, we took into consideration all the sources of anisotropy in the energy shift of the Landau level situated below the quasitransverse phonon continuum. We believe that for this type of material (anisotropic, uniaxial, and with the dielectric function described by a two-oscillator model) the extension of such an analysis to other domains of energy (using the so-called memory function approach[30]) will show the possibility of existence of an intermediate magnetopolaron branch situated in the domain

$$(\hbar\omega_{\mathrm{TO},h}+\hbar\omega/2+\Delta E_0^{RSPT},\hbar\omega_{\mathrm{LO,l}}+\hbar\omega/2+\Delta E_0^{RSPT}),$$

$\omega_{\mathrm{TO},h}$, and $\omega_{\mathrm{LO},l}$ being the highest transverse optical phonon frequency and the lowest longitudinal optical phonon frequency, respectively.

For anisotropic polar crystals with complex structure it would be thus possible to find additional intermediate branches of the magnetopolaron spectrum, which have to play an important role in the cyclotron resonance phenomenon in such materials.

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