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Complex magneto-polaron spectrum of the layer compound InSe

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Abstract

We analyse the energy magneto-polaron spectrum of the polar uniaxial layer compound InSe in a magnetic field directed along the optical axis. A quasi-bidimensional behaviour of the electron gas in this particular structure was considered. In the framework of the Wigner–Brillouin perturbational theory we systematically take into account all the sources of anisotropy. We found that the implied anisotropy brings distinctive contributions to the complex energy magneto-polaron spectrum of polar uniaxial crystals. The theory is used to examine the experimental results obtained from cyclotron resonance frequency measurements in InSe at low temperature.

1. Introduction

Based on measurements of cyclotron resonance and Shubnikov–de Hass oscillations at low temperatures, Portal and co-workers [1] proved an apparently two-dimensional (2D) behaviour of the electron gas in bulk InSe. Consequently, it was considered [2] that in n-type material, during the growth of the crystal, the shallow donor impurities are accumulated at the defect planes leading to the formation of several sheets with a low individual estimated electron density (of order 1×10^{11} cm^{-2}). Subsequent cyclotron studies [3, 4] have confirmed the proposed electron gas model. An improvement [5] of this model was done by considering a quasi-two-dimensional (Q2D) behaviour of the electron gas. Thus, in the absence of knowledge of the confining potential along the optical axis, the finite extent of the electron wavefunction in the symmetric plane layer is taken into account by considering [5] a wavefunction $|\varphi(z)|^2 \sim \mathrm{e}^{-|z|/a}$, a being a fitting parameter.

In uniaxial polar crystals, the optical-phonon-mode frequencies, $\omega_\mu(\theta)$ (μ and θ being the branch index and the angle between the phonon wavevector and the optical axis, respectively), depend on the propagation direction [6]. For the particular case of InSe it was found [7] that the extraordinary phonon modes can be classified as quasi-transverse-modes having the frequencies $\omega_1(\theta)$ in the domain $[\omega_{\mathrm{TO}}^{\perp}, \omega_{\mathrm{TO}}^{\parallel}]$ and quasi-longitudinal modes with the frequencies $\omega_2(\theta)$ in $[\omega_{\mathrm{LO}}^{\parallel}, \omega_{\mathrm{LO}}^{\perp}]$. The frequencies $\omega_{\mathrm{TO}}^{\parallel,(\perp)}$ and $\omega_{\mathrm{LO}}^{\parallel,(\perp)}$ are the frequencies of

the transverse/longitudinal phonon modes along the principal directions, and they verify the inequalities $\omega_{\mathrm{LO}}^{\perp} > \omega_{\mathrm{LO}}^{\parallel} > \omega_{\mathrm{TO}}^{\parallel} > \omega_{\mathrm{TO}}^{\perp}$. The symbols $\perp$ and $\parallel$ correspond to a direction that is either orthogonal or parallel to the optical axis.

A general method to obtain an equivalent form of the Fröhlich Hamiltonian extended to the anisotropic crystals having complex basis (with the uniaxial case written explicitly) was developed in [8]. The same electron–optical-phonon interaction Hamiltonian was used [9] to discuss the electron–optical-phonon scattering in wurtzite crystals, particularly for GaN. Solving the problem of the optical polaron in uniaxial crystals [8], the forms of the self-energy and the effective-mass tensor are found to depend on the quantities $\alpha_{\mu}(\theta)$ which are extensions to the uniaxial case of the dimensionless Fröhlich coupling constant α.

Because of their important effects on the magneto-polaron spectrum and, consequently, on the cyclotron resonance phenomenon in a polar uniaxial crystal, the anisotropic properties of the system have to be properly taken into account. Contributions of all the sources of the system's anisotropy (the shape of constant-energy surfaces of the bare electron, the electron–optical-phonon interaction and the frequency spectrum of the extraordinary phonon modes) to the energy levels of a 3D magneto-polaron (belonging to the lower magneto-polaron branch) have been considered in [10] in the context of the 'improved Wigner–Brillouin perturbational theory' [11] (IWBPT). For InSe it was shown [10] that the polaron coupling function $\alpha_1(\theta)$ for the quasi-transverse phonon modes is small compared to that for the quasi-longitudinal modes. However, the presence of the continuum frequency distribution of the quasi-transverse modes in a domain bellow that of the quasi-longitudinal modes plays an important role in the cyclotron resonance (implying the magneto-polaron levels of the lower branch) at high magnetic fields.

The model in [5], which uses the so-called 'memory-function method' [12] to derive the appropriate component of the magneto-conductivity tensor, had successfully explained the results of the cyclotron resonance measurements performed at low temperatures in InSe, but the anisotropic properties of the system were taken into account in a simplified manner. Thus, instead of the entire spectrum of the extraordinary phonon modes, discussed above, only a phonon frequency, ω_{LO}, was considered [5], as in the isotropic case. Moreover, the two anisotropic polaron couplings $\alpha_{\perp}$ and $\alpha_{\parallel}$ for the perpendicular and parallel motions to the optical axis were introduced instead of the right polaron coupling 'functions' $\alpha_{\mu}(\theta)$ [8, 10, 13].

We shall discuss here the effects of the anisotropic properties of the system and the finite z-extent of the electron wavefunction on the cyclotron resonance at low temperature in a polar uniaxial semiconductor placed in a dc magnetic field directed along the optical axis. In order to observe the direct influence of the peculiar anisotropic properties of the phonon spectrum on the cyclotron resonance we chose to get the entire magneto-polaron spectrum instead of using the memory-function approach. By considering in the proper way all the involved anisotropies we reveal new splittings in the magneto-polaron spectrum of a system having a complex phonon spectrum.

2. Hamiltonian and perturbational calculation

In the presence of a dc magnetic field $\mathbf{B}_0$ directed along the optical axis of the crystal (parallel to the z-axis), the Hamiltonian of a bare electron is written in the Coulomb gauge as

$$H_{\mathrm{e}} = \hbar\omega_{\mathrm{c}}(A^{+}A + 1/2) + \frac{p_z^2}{2m_{\parallel}} + V(z), \tag{1}$$

where the harmonic oscillator operators A and A^{+} (later there will also be B and B^{+}) are introduced [10, 14, 15] to describe the transverse part of the electron Hamiltonian and the

unperturbed electron state. In equation (1), $\omega_c = eB_0/m_\perp$ is the cyclotron frequency of the bare electron for the magnetic field parallel to the optical axis, $m_\perp$ and $m_\parallel$ being the diagonal components of the bare electron effective mass-tensor. $V(z)$ and p_z are the confining potential and the component of the electron momentum along the optical axis, respectively. Considering the interaction of a conduction electron with the optical phonons, the Hamiltonian of the system becomes

$$H = H_e + \sum_{\vec{q},\mu}\left(\frac{V_\mu(\vec{q})}{\sqrt{V}} b_{\vec{q},\mu} e^{i\vec{q}\cdot\vec{r}} + \text{H.c.}\right) + \sum_{\vec{q},\mu} \hbar\omega_\mu(\vec{q}) b^+_{\vec{q},\mu} b_{\vec{q},\mu}, \tag{2}$$

where $b^+_{\vec{q},\mu}$ and $b_{\vec{q},\mu}$ are, respectively, creation and annihilation operators for a phonon with wavevector $\vec{q}$, branch index μ, and frequency $\omega_\mu(\vec{q})$; V is the volume of the system. The form of the coupling constants $V_\mu(\vec{q})$ has been previously obtained by Toyozawa [16] and used in [8] to discuss the properties of the anisotropic uniaxial polaron.

Denoting by $\varphi_l = \langle z|l\rangle$ and E_l the wavefunction describing the motion of the bare electron in the confining potential $V(z)$ and, respectively, its corresponding energy, the second-order energy correction of the unperturbed state, $|\Psi_i\rangle = |n, m, l\rangle \otimes |0\rangle_{ph} = |n\rangle_A \otimes |m\rangle_B \otimes |l\rangle \otimes |0\rangle_{ph}$, has the form

$$\Delta E_{n,l} = -\frac{1}{V}\sum_{\vec{q},\mu} |V_\mu(\vec{q})|^2 \sum_{n',m',l'} \frac{|\langle n, m, l|e^{i\vec{q}\cdot\vec{r}}|n', m', l'\rangle|^2}{\hbar\omega_c(n'-n) - \Delta_{n,l} + E_{l'} - E_l + \hbar\omega_\mu(\vec{q})}. \tag{3}$$

Here $|n\rangle_A$ and $|m\rangle_B$ are the oscillator states $(n!)^{-1/2}(A^+)^n|0\rangle_A$ and $(m!)^{-1/2}(B^+)^m|0\rangle_B$, with $|0\rangle_A$ and $|0\rangle_B$ the vacuum states of the operators A and B, $|0\rangle_{ph}$ being the phonon vacuum state.

In the context of the IWBPT $\Delta_{n,l} = \Delta E_{n,l} - \Delta E^{RSPT}_{0,l_0}$, where the upper index RSPT means that the corresponding quantity is calculated in the frame of the Rayleigh–Schrödinger perturbation theory, l_0 being the quantum number of the fundamental state describing the z-motion of the electron. Generally, for $\Delta E^{RSPT}_{n,l}$, a form similar to (3) but with $\Delta_{n,l} = 0$ is used.

Working at zero temperature and considering that the energies of the excited states for z-motion are large relative to the in-plane (x, y) energies, we shall restrict ourselves to the contribution of the fundamental state $|l_0\rangle$. In this limit, the expression (3) of the energy correction becomes

$$\Delta E_{n,l_0} = -\frac{1}{V}\sum_{\vec{q},\mu} |V_\mu(\vec{q})|^2 \sum_{n',m'} \frac{|\langle n, m|e^{i\vec{q}_\perp\cdot\vec{\rho}}|n', m'\rangle|^2 |\langle l_0|e^{iq_z z}|l_0\rangle|^2}{\hbar\omega_c(n'-n) - \Delta_{n,l_0} + \hbar\omega_\mu(\vec{q})}, \tag{4}$$

$\vec{\rho}$ and $\vec{q}_\perp$ having x- and y-components only. This formula would be directly obtained if a form of an appropriate effective Hamiltonian [17] is used from the beginning. In the context of such an approximation the results are improved by considering $\varphi_{l_0}(z)$ as a variational wavefunction [5, 17].

The finite z-extent of the electron wavefunction in the symmetrical planar layer is taken into account here by using two forms for the trial wavefunction $\varphi_{l_0}(z)$: one which verifies

$$|\varphi^{(1)}_{l_0}(z)|^2 = (2a)^{-1} e^{-|z|/a}, \tag{5}$$

(also considered in [5]) and the other being of Gaussian type,

$$\varphi^{(2)}_{l_0}(z) = (\sqrt{\pi}a)^{-1/2} e^{-z^2/(2a^2)}. \tag{6}$$

Based on the assumption that the behaviour of the function in the vicinity of the point $z = 0$ plays an unimportant role in the fitting process of the experimental results, the first form of the wavefunction, though not differentiable at $z = 0$, has been previously [5] used. We used two such different forms in order to observe how sensitive the final results are to the particular shape of the chosen wavefunctions.

3. Lower magneto-polaron branch

This magneto-polaron branch is constituted by the Landau levels situated, due to the magneto-polaron splitting, below the optical-phonon continuum. We consider here the entire optical phonon spectrum (including the quasi-transverse modes). In this case all the denominators of equation (4) are positive, so the summation over the intermediate states $|n', m'\rangle$ can be performed [12] paying the price of introducing a supplemental τ-integral:

$$\Delta E_{n,l_0,j} = -\sum_{\vec{q},\mu} \frac{|V_\mu(\vec{q})|^2}{\hbar V} f_j(q_z) \int_0^\infty \mathrm{d}\tau\, \mathrm{e}^{-[\omega_\mu(\vec{q})-\Delta^{(\mathrm{low})}_{n,l_0,j}/\hbar]\tau} \langle n, m|\mathrm{e}^{\mathrm{i}\vec{q}_\perp\cdot\vec{\rho}(\tau)}\mathrm{e}^{-\mathrm{i}\vec{q}_\perp\cdot\vec{\rho}(0)}|n, m\rangle, \quad (7)$$

where

$$\vec{\rho}(\tau) = \mathrm{e}^{H_\mathrm{e}\tau/\hbar}\vec{\rho}\mathrm{e}^{-H_\mathrm{e}\tau/\hbar} \quad (8)$$

and

$$f_j(q_z) = \left|\int_{-\infty}^{+\infty} \mathrm{d}z\, \varphi^{(j)*}_{l_0}(z)\mathrm{e}^{\mathrm{i}q_z z}\varphi^{(j)}_{l_0}(z)\right|^2. \quad (9)$$

In terms of A and B operators the exponential $\mathrm{e}^{\mathrm{i}\vec{q}_\perp\cdot\vec{\rho}}$ can be put into the form [15]

$$\mathrm{e}^{\mathrm{i}\vec{q}_\perp\cdot\vec{\rho}} = L^+_{\vec{q}} M^+_{\vec{q}}, \quad (10)$$

where

$$L_{\vec{q}} = \exp\left\{\left(\frac{\hbar}{2m_\perp\omega_\mathrm{c}}\right)^{1/2}(q_+A - q_-A^+)\right\}, \quad (11)$$

$$M_{\vec{q}} = \exp\left\{-\mathrm{i}\left(\frac{\hbar}{2m_\perp\omega_\mathrm{c}}\right)^{1/2}(q_+B^+ + q_-B)\right\}, \quad (12)$$

and

$$q_\pm = q_x \pm \mathrm{i}q_y. \quad (13)$$

The operators B and B^+ used here differ from those of [15] by a phase factor, with no consequence of subsequent developments. Because the operators B and B^+ are not presented in the Hamiltonian H_e, the expression of the density–density correlation function appearing in (7) is independent of the quantum number m [12]:

$$\langle n|L^+_{\vec{q}}(\tau)L_{\vec{q}}(0)|n\rangle = \exp\left[-\frac{\hbar q_\perp^2}{2m_\perp\omega_\mathrm{c}}(1-\mathrm{e}^{-\omega_\mathrm{c}\tau})\right]\sum_{p=0}^{n}\frac{C(n,p)}{p!}\left[\frac{2\hbar q_\perp^2}{m_\perp\omega_\mathrm{c}}\sinh^2\left(\frac{\omega_\mathrm{c}\tau}{2}\right)\right]^p, \quad (14)$$

with $C(n, p)$ being the combinations.

Thus, the expression (7) of the energy correction of the n-Landau level belonging to the lower magneto-polaron branch becomes

$$\Delta E^{(\mathrm{low})}_{n,l_0,j}/\hbar = -\frac{2}{\pi\sqrt{\omega_\mathrm{c}}}\sum_\mu \int_0^{\pi/2}\mathrm{d}\theta\, \omega_\mu^{3/2}(\theta)\alpha_\mu^{2D}(\theta)\sum_{p=0}^{n}C(n,p)\frac{2^{2p}}{p!}\int_0^\infty \frac{\mathrm{d}t}{\sqrt{1-\mathrm{e}^{-t}}}$$
$$\times \exp\left[-\frac{\omega_\mu(\theta)-\Delta^{(\mathrm{low})}_{n,l_0,j}/\hbar}{\omega_\mathrm{c}}t\right]\left[\frac{\sinh^2(t/2)}{1-\mathrm{e}^{-t}}\right]^p J^{(j)}_p(\theta,t), \quad (15)$$

where by $J^{(j)}_p$ we have denoted the integral over q determined by $f_j(q_z)$,

$$J^{(j)}_p(\theta,t) = J^{(j)}_p(\beta) = \int_0^\infty \mathrm{d}x\, f_j(\beta,x)x^{2p}\mathrm{e}^{-x^2}. \quad (16)$$

For the two considered trial wavefunctions, the $f_j(\beta)$ have the form

$$f_1(\beta, x) = \beta^4(\beta^2 + x^2)^{-2}, \tag{17}$$

$$f_2(\beta, x) = \exp\left(-\frac{x^2}{2\beta^2}\right), \tag{18}$$

with

$$\beta^2 = \frac{\hbar}{2m_\perp \omega_c a^2}(1 - e^{-t}) \tan^2\theta. \tag{19}$$

For the two selected cases, the integral over x can be exactly performed, obtaining

$$J_p^{(1)}(\beta) = \frac{\Gamma(p + 1/2)}{2}\beta^{p+3/2}e^{\beta^2}W_{-p/2-3/4,\,p/2-3/4}(\beta^2), \tag{20}$$

$$J_p^{(2)}(\beta) = \frac{\Gamma(p + 1/2)}{2}\frac{\beta^{2p+1}}{(\beta^2 + 1/2)^{p+1/2}}, \tag{21}$$

$\Gamma(z)$ and $W_{\mu,\nu}(z)$ being the gamma and Whittaker function, respectively. In equation (15), instead of the 3D-polaronic coupling function $\alpha_\mu(\theta)$ we used the corresponding 2D form, previously introduced in [10],

$$\alpha_\mu^{2D}(\theta) = \sin\theta \lim_{m_\parallel \to \infty} \alpha_\mu(\theta) = \frac{m_\perp^{1/2} q^2 |V_\mu(\vec{q})|^2}{\pi\hbar[2\hbar\omega_\mu(\theta)]^{3/2}}. \tag{22}$$

It is worth noting that in the limit of a 2D electron gas ($a \to 0$), both considered functions $f_j(\beta, x)$ reach unity. Then, performing the integration over x and t variables, equation (15) reduces to equation (23) of [10]. However, the approximation considered before by which only the state $|l_0\rangle$ of the lowest energy was taken into account, disregarding the contributions of all the states $|l\rangle$ having higher energies, prevents the achievement of the 3D result in the limit $a \to \infty$.

At zero temperature, the cyclotron resonance frequency of the lower magneto-polaron branch, defined through the energy difference between $E^{(\mathrm{low})}_{1,l_0,j}$ and $E_{0,l_0,j}$, is obtained by using the corresponding expressions for the energy shift:

$$\hbar\Omega_j^{(\mathrm{low})} = \hbar\omega_c + \Delta E^{(\mathrm{low})}_{1,l_0,j} - \Delta E_{0,l_0,j}. \tag{23}$$

In the above equation, $\Delta E_{0,l_0,j}$ is the term with $n = 0$ of equation (15).

4. Upper magneto-polaron branch

The upper magneto-polaron branch contains all magneto-polaron levels $E_{n.l_0}$ situated in the plane (E, B_0) above the curve $E_{0,l_0} + \hbar\omega_{\mathrm{LO}}^{\perp}$; $\omega_{\mathrm{LO}}^{\perp}$ is the maximum frequency of the phonon spectrum. The energy correction of the n-Landau level of the upper magneto-polaron branch is also given by equation (4). However, this time, the denominators $D_{n',n} = \omega_c(n'-n) - \Delta^{(\mathrm{upp})}_{n,l_0,j}/\hbar + \omega_\mu(\theta)$ are negative for $n' < n$. Thus, in order to perform the summation over the intermediate states by introducing a supplemental τ-integral, equation (4) has to be arranged accordingly to the form proposed by Larsen in [15]:

$$\begin{aligned}\Delta E^{(\mathrm{upp})}_{n,l_0,j} = &-\frac{1}{\hbar V}\sum_{\vec{q},\mu}|V_\mu(\vec{q})|^2 f_j(q_z) \\ &\times\left(\sum_{n',m'}\frac{|\langle n, m|L_{\vec{q}}^{+}M_{\vec{q}}^{+}|n', m'\rangle|^2}{D_{n',n}} - \sum_{n'<n,m'}\frac{|\langle n, m|L_{\vec{q}}^{+}M_{\vec{q}}^{+}|n', m'\rangle|^2}{D_{n',n}}\right) \\ &-\frac{1}{\hbar V}\sum_{\vec{q},\mu}|V_\mu(\vec{q})|^2 f_j(q_z)\sum_{n'<n,m'}\frac{|\langle n, m|L_{\vec{q}}^{+}M_{\vec{q}}^{+}|n', m'\rangle|^2}{D_{n',n}}.\end{aligned} \tag{24}$$

Then, the expression entering the curly brackets, denoted by T, can be written as

$$T = \sum_{n',m'} \int_0^\infty \mathrm{d}\tau\, \mathrm{e}^{-D_{n',n}\tau} |\langle n, m|L_{\vec{q}}^{+} M_{\vec{q}}^{+}|n', m'\rangle|^2 - \sum_{n'<n,m'} \int_0^\infty \mathrm{d}\tau\, \mathrm{e}^{-D_{n',n}\tau} |\langle n, m|L_{\vec{q}}^{+} M_{\vec{q}}^{+}|n', m'\rangle|^2. \tag{25}$$

Of course, the τ-integrals of the terms with $n' < n$ are divergent at the upper limit, but their total contribution at T is zero. Then, using the completeness of the states $|n'\rangle \otimes |m'\rangle$, the form (25) becomes

$$T = \int_0^\infty \mathrm{d}\tau \exp\left[-(\omega_\mu(\vec{q}) - \Delta_{n,l_0,j}^{(\mathrm{upp})}/\hbar)\tau\right] \left\{ \langle n|L_{\vec{q}}^{+}(\tau) L_{\vec{q}}^{+}(0)|n\rangle - \sum_{n'<n} \mathrm{e}^{(n-n')\omega_\mathrm{c}} |\langle n|L_{\vec{q}}^{+}|n'\rangle|^2 \right\}, \tag{26}$$

where the square of the matrix element has the form [18]

$$|\langle n|L_{\vec{q}}^{+}|n'\rangle|^2 = \frac{n'!}{n!} \left(\frac{\hbar q_\perp^2}{2m_\perp \omega_\mathrm{c}}\right)^{n-n'} \left[L_{n'}^{n-n'}\left(\frac{\hbar q_\perp^2}{2m_\perp \omega_\mathrm{c}}\right)\right]^2 \exp\left[-\frac{\hbar q_\perp^2}{2m_\perp \omega_\mathrm{c}}\right]. \tag{27}$$

$L_{n'}^{n-n'}(z)$ are the associated Laguerre polynomials defined by the equation [19]

$$L_{n'}^{n-n'}(z) = \sum_{j=0}^{n'} \frac{(-1)^j C(n, n'-j)}{j!} z^j. \tag{28}$$

The final expression of the energy correction to the n-Landau level of the upper magneto-polaron branch can be put into the form

$$\begin{aligned}\Delta E_{n,l_0,j}^{(\mathrm{upp})}/\hbar = &-\frac{2}{\pi\sqrt{\omega_\mathrm{c}}} \sum_\mu \int_0^{\pi/2} \mathrm{d}\theta\, \alpha_\mu^{2\mathrm{D}}(\theta) \omega_\mu^{3/2}(\theta) \int_0^\infty \mathrm{d}t \exp\left[-\frac{\omega_\mu(\theta) - \Delta_{n,l_0,j}^{(\mathrm{upp})}/\hbar}{\omega_\mathrm{c}} t\right] \\ &\times \left\{ \sum_{p=0}^{n} C(n, p) \frac{2^{2p}}{p!} \frac{1}{\sqrt{1-\mathrm{e}^{-t}}} \left[\frac{\sinh^2(t/2)}{1-\mathrm{e}^{-t}}\right]^p J_p^{(j)}(\theta, t) \right. \\ &\left. - \sum_{n'<n} \mathrm{e}^{-(n'-n)t} \frac{n'!}{n!} J_{n,n'}^{(j)}(\beta^\infty) \right\} - \frac{2\sqrt{\omega_\mathrm{c}}}{\pi} \sum_\mu \int_0^{\pi/2} \mathrm{d}\theta\, \alpha_\mu^{2\mathrm{D}}(\theta) \omega_\mu^{3/2}(\theta) \\ &\times \sum_{n'<n} \frac{n'!}{n!} \frac{J_{n,n'}^{(j)}(\beta^\infty)}{\omega_\mathrm{c}(n'-n) - \Delta_{n,l_0,j}^{(\mathrm{upp})}/\hbar + \omega_\mu(\theta)},\end{aligned} \tag{29}$$

where we have denoted

$$J_{n,n'}^{(j)}(\beta^\infty) = \int_0^\infty \mathrm{d}x\, f_j(\beta^\infty, x) \mathrm{e}^{-x^2} (x^2)^{n-n'} [L_{n'}^{n-n'}(x^2)], \tag{30}$$

with β^∞ being the value of β for $t \to \infty$.

Taking into account equation (28) of the associated Laguerre polynomials, the integral (30) can be performed and the result is a linear combination of integrals (20) and (21) written for $t \to \infty$, for any of the two considered functions f_j. For the sake of simplicity we shall not present these expressions here.

The cyclotron resonance frequency for the upper magneto-polaron branch is given by

$$\Omega_j^{(\mathrm{upp})} = \omega_\mathrm{c} + \Delta E_{1,l_0,j}^{(\mathrm{upp})}/\hbar - \Delta E_{0,l_0,j}/\hbar. \tag{31}$$

For the particular case of an isotropic 2D magneto-polaron ($a \to 0$) and considering the RSPT context ($\Delta_{0,l_0,j}^{(\mathrm{upp})} = 0$), equation (31) reduces to equation (14) of [14].

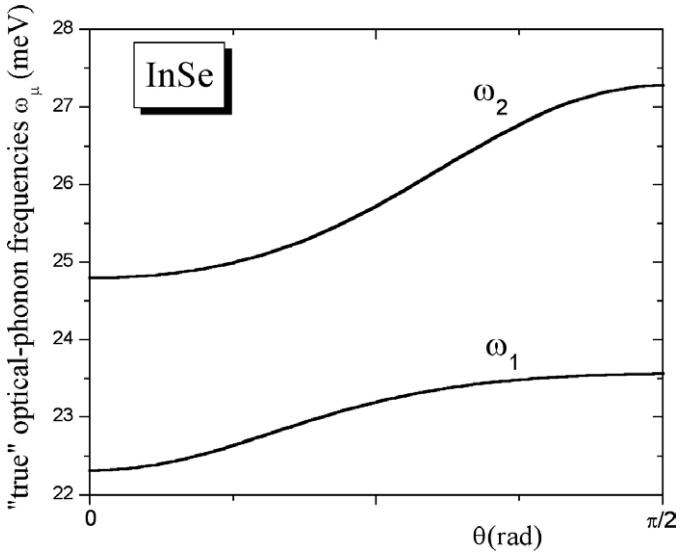

Figure 1. The angular dependence of the 'true' optical-phonon modes $\omega_\mu(\mu = 1, 2)$ in layer compound InSe.

5. Intermediate magneto-polaron branch

The appearance of this branch of the magneto-polaron energy spectrum, never stated before, is a consequence of the properties of the optical phonon spectrum, directly related to the involved anisotropy. Thus, for InSe, a material which presents only two branches of extraordinary phonon spectrum ($\mu = 1, 2$), the intermediate magneto-polaron branch has the character of a lower branch for the quasi-longitudinal phonon modes ($\mu = 2$) and, at the same time, that of an upper branch for the quasi-transverse phonon modes ($\mu = 1$).

Denoting the expressions (29) and (15) written for $\mu = 1$ and 2 by $\Delta E^{(\mathrm{upp})}_{n,l_0,j}(\mu = 1)$ and $\Delta E^{(\mathrm{low})}_{n,l_0,j}(\mu = 2)$, respectively, the expression of the energy shift of the n-Landau level of the intermediate magneto-polaron branch can be formally put into the form

$$\Delta E^{(\mathrm{int})}_{n,l_0,j} = \Delta E^{(\mathrm{upp})}_{n,l_0,j}(\mu = 1) + \Delta E^{(\mathrm{low})}_{n,l_0,j}(\mu = 2), \tag{32}$$

with a unique quantity $\Delta^{(\mathrm{int})}_{n,l_0,j}$ entering in both terms of the right member of the above equation.

The presence of such an intermediate magneto-polaron branch introduces into the cyclotron resonance spectrum a new frequency:

$$\Omega^{(\mathrm{int})}_{l_0,j} = \omega_c + \Delta E^{(\mathrm{int})}_{1,l_0,j}/\hbar - \Delta E_{0,l_0,j}/\hbar. \tag{33}$$

A direct generalization to the case of a uniaxial crystal having many extraordinary phonon branches leads to the appearance of other supplemental intermediate magneto-polaron branches.

6. Results and discussion

In figure 1 we show the angular dependence of the optical phonon mode frequencies belonging to the quasi-transverse branch for $\mu = 1$ and quasi-longitudinal branch for $\mu = 2$, respectively. To allow a better interpretation of the experimental results, the nonparabolicity of the electron

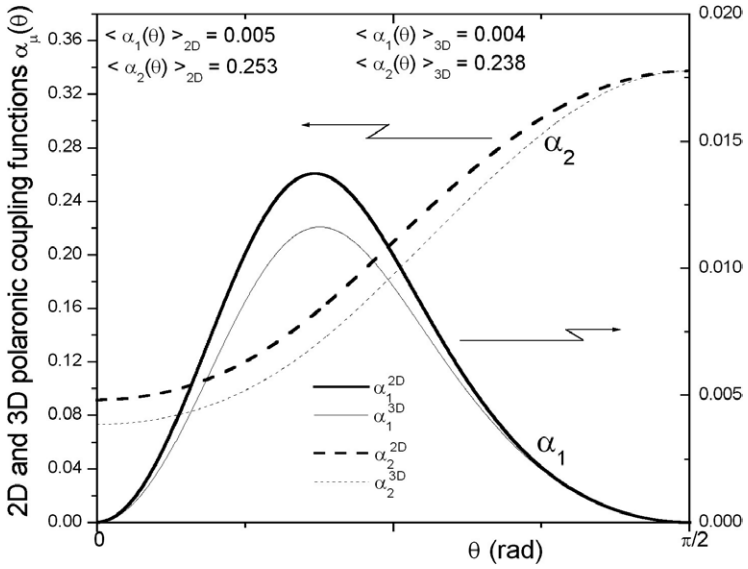

Figure 2. The angular dependence of the polaronic coupling functions α_μ (quasi-transverse branch $\mu = 1$ (right axis), and quasi-longitudinal branch $\mu = 2$ (left axis)) for InSe in 2D and 3D cases ($m_\perp = 0.127\ m_0$; $m_\parallel = 0.081\ m_0$); the symbol $\langle\,\rangle$ means angular average.

energy band (without polaron effect) which is almost a linear function of the magnetic field strength [20] is considered. Thus, according to [5], a small additional mass increase of 0.14% T^{-1} was taken into account in the following. This effect leads to a small dependence on the magnetic field strength of the polaronic coupling functions $\alpha_\mu^{2D}(\theta)$. In figure 2, the two functions $\alpha_\mu^{2D}(\theta)$ for the 2D case and $\alpha_\mu^{3D}(\theta)$ for the 3D case ($\mu = 1, 2$) are presented in the absence of a magnetic field. The difference in the angular dependence of 2D and 3D polaronic coupling functions is given by equation (39).

To compare the results of our calculation to the experimental measurements [5] we used only two fitting parameters, $m_\perp$ and a. The phonon spectrum and the electron-optical phonon coupling functions are entirely determined from the experiment [7, 21]. As is well known, the effective mass of the bare electron (the effective mass tensor for the anisotropic case) is determined by fitting the dependence on the magnetic field of the cyclotron resonance frequency, especially (for technical reasons) in the domain of weak magnetic fields. This fitting procedure has a self-consistent character because the polaronic constants α^{2D} (the polaronic functions $\alpha_\mu^{2D}(\theta)$ for the uniaxial case) depend on $m_\perp$. In [5], the value 0.131 m_0 for $m_\perp$, determined before [3], was considered from the beginning. Also, considering very schematically the phonon spectrum and the electron–phonon interaction, in analysing the experimental results, all the quantities ω_{LO}, $\alpha_\perp$, $\alpha_\parallel$, and a [5] seem to play a fitting-parameter character. Here, benefiting from the experimental results concerning the behaviour of the cyclotron frequency in a large domain of magnetic fields we considered $m_\perp$ as a fitting parameter.

In figure 3 we show the first Landau levels ($n = 0, 1, 2$) of the magneto-polaron spectrum obtained for the parameters $m_\perp = 0.127\ m_0$ and $a = 37.5$ Å, with the first electron wavefunction $\varphi_{l_0}^{(1)}(z)$, parameters which assure the best fit of the cyclotron resonance spectrum (see figure 5). As a direct consequence of the optical-phonon spectrum of this uniaxial crystal a supplemental branch of the magneto-polaron spectrum, called the intermediate branch, appears.

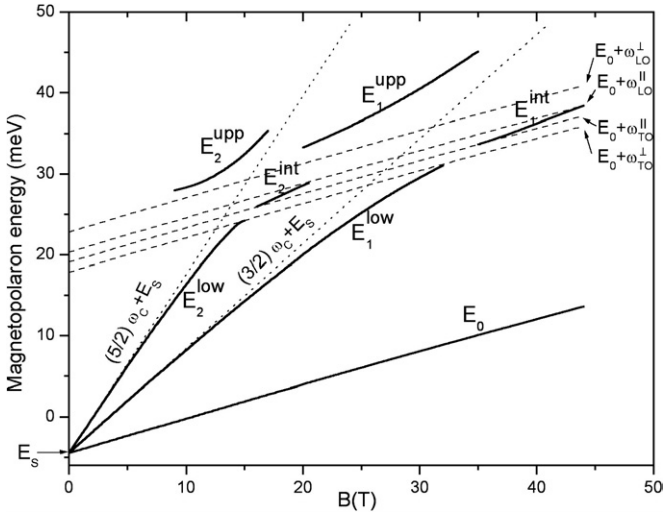

Figure 3. The first Landau levels ($n = 0$, 1, and 2) of the magneto-polaron spectrum (thick solid lines) for InSe in the Q2D case with the first trial electron wavefunction, $\varphi_{l_0}^{(1)}$ ($a = 37.5$ Å).

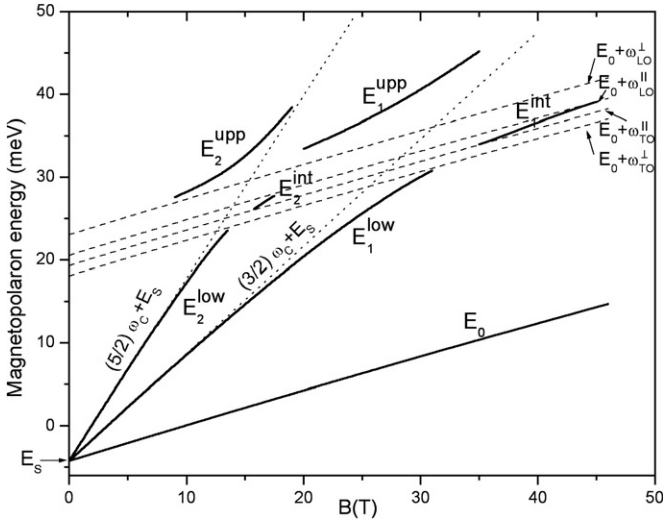

Figure 4. The first Landau levels ($n = 0$, 1, and 2) of the magneto-polaron spectrum (thick solid lines) for InSe in Q2D case with the second trial electron wavefunction, $\varphi_{l_0}^{(2)}$ ($a = 75$ Å).

Though it is situated at unexplored high magnetic fields, this new intermediate magneto-polaron branch follows naturally from the involved anisotropy of a system with a complex phonon spectrum. The value of the parameter a is very close to the value ($a = 36$ Å) obtained in [5].

In figure 4 are shown the same results as before, but now using the second form of the electron wavefunction and the parameters $m_\perp = 0.127\, m_0$ and $a = 75$ Å.

In figure 5 the experimental data [5] (solid dots on graph) are fitted with the corresponding expressions of the cyclotron resonance frequencies belonging to the different branches, for the first electron wavefunction (the solid lines) and for the second electron wavefunction (the dotted

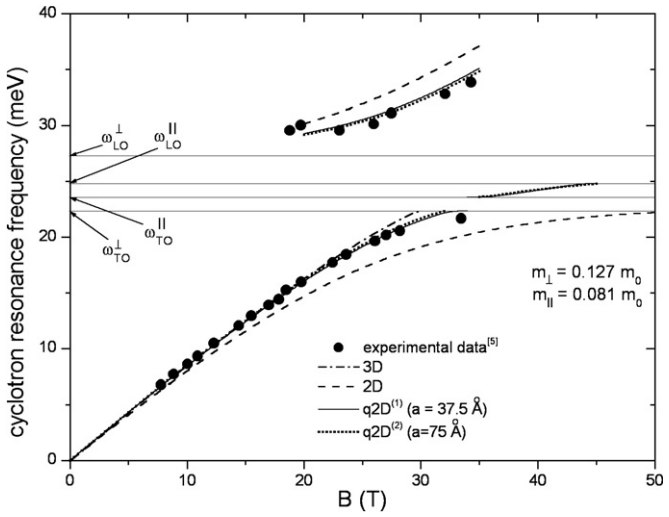

Figure 5. Cyclotron resonance frequencies versus the magnetic field for InSe considering a 3D (dash–dot line), 2D (dashed line), and Q2D behaviour (solid line—$\varphi_{l_0}^{(1)}$; dotted line—$\varphi_{l_0}^{(2)}$). Besides the lower and the upper branches, a new intermediate magneto-polaron branch is calculated at higher magnetic fields.

lines). Though the two values of the parameter a which realize the best fit are substantially different for the two considered electron wavefunctions, the width of the Q2D electron layer defined as $w = \langle (z - \langle z \rangle)^2 \rangle^{1/2}$ has, approximately, the same value in both cases, 52 Å. Therefore, the results seem to depend merely on the width of the Q2D electron gas and not on the particular form of the variational wavefunction.

As follows from the magneto-polaron spectrum calculations, we believe that for large magnetic fields there is a supplemental branch of cyclotron resonance frequencies in the spectral domain $[\omega_{TO}^{\parallel}, \omega_{LO}^{\parallel}]$.

Now, returning to the magneto-polaron energy spectrum figures 3 and 4, we remark that the Landau levels of the lower branch, for $B_0 \to 0$, reach a value that, instead of being between the 3D polaron self-energy E_S (−6.47 meV) and its corresponding 2D-value (−8.93 meV), is higher than the 3D polaron self-energy. This is a direct consequence of the fact that, not knowing the confining potential, we have to restrict ourselves to the contribution of the fundamental state $|l_0\rangle$. However, choosing the second form of the electron wavefunction to be of Gaussian type (which means a potential for a harmonic oscillator) we have the possibility to evaluate exactly the contribution to the energy correction of all the intermediate states (at least for the lower magneto-polaron branch).

In this case, equation (7) becomes

$$\Delta E_{n,l_0} = -\sum_{\vec{q},\mu} \frac{|V_\mu(\vec{q})|^2}{\hbar V} \int_0^\infty \mathrm{d}\tau\, \mathrm{e}^{-[\omega_\mu(\vec{q}) - \Delta_{n,l_0}^{(\mathrm{low})}/\hbar]\tau} \langle n, m, l_0 | \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}(\tau)} \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{r}(0)} | n, m, l_0 \rangle, \qquad (34)$$

where $\vec{r}$ and $\vec{q}$ have also z-component.

Now, the density–density correlation function factorizes:

$$\langle n, m, l_0 | \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}(\tau)} \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{r}(0)} | n, m, l_0 \rangle = \langle l_0 | \mathrm{e}^{\mathrm{i}q_z z(\tau)} \mathrm{e}^{-\mathrm{i}q_z z(0)} | l_0 \rangle \langle n, m | \mathrm{e}^{\mathrm{i}\vec{q_\perp}\cdot\vec{\rho}(\tau)} \mathrm{e}^{-\mathrm{i}\vec{q_\perp}\cdot\vec{\rho}(0)} | n, m \rangle, \qquad (35)$$

the last factor being calculated before. The first factor of equation (35) can be directly

calculated, obtaining

$$\left\langle l_0 \left| e^{iq_z z(\tau)} e^{-iq_z z(0)} \right| l_0 \right\rangle = \exp\left[-\frac{q_z^2 a^2}{2} \left(1 - \exp\left(-\frac{\hbar \tau}{m_\parallel a^2} \right) \right) \right]. \tag{36}$$

Taking into account equations (14) and (36), and performing the integrals over the azimuthal angle and the modulus of the phonon wavevector, the expression (34) of the energy correction becomes

$$\Delta E_{n,l_0}/\hbar = -\frac{1}{\sqrt{\pi}\omega_c} \sum_\mu \int_0^{\pi/2} d\theta \sin\theta \omega_\mu^{3/2}(\theta) \alpha_\mu^{2D}(\theta) \int_0^\infty dt \exp\left[-\frac{\omega_\mu(\theta) - \Delta_{n,l_0}/\hbar}{\omega_c} t \right]$$
$$\times \sum_{p=0}^{n} C(n,p) \frac{(2p-1)!!}{p!} \left[\frac{2\sin^2\theta}{Z_a(t,\theta)} \sinh^2(t/2) \right]^p \frac{1}{\sqrt{Z_a(t,\theta)}}, \tag{37}$$

where

$$Z_a(t,\theta) = \frac{m_\perp \omega_c a^2}{\hbar} \left(1 - \exp\left(-\frac{\hbar t}{m_\parallel a^2 \omega_c} \right) \right) \cos^2\theta + (1 - e^{-t}) \sin^2\theta. \tag{38}$$

Now, taking the limit $a \to \infty$ and considering the relationship between the polaronic coupling functions $\alpha_\mu(\theta)$ for the case 2D and 3D,

$$\alpha_\mu^{2D}(\theta) = m_\perp^{1/2} \left(\frac{\cos^2\theta}{m_\parallel} + \frac{\sin^2\theta}{m_\perp} \right)^{1/2} \alpha_\mu^{3D}(\theta), \tag{39}$$

equation (37) reduces to the expression of the energy correction (16) of [10], obtained in the 3D case, but written for $p_z = 0$; p_z is the eigenvalue of the free-electron momentum along the z-axis. Of course, the limit $a \to 0$ leads to the 2D case.

In figure 6 the first two Landau levels of the lower magneto-polaron branch are shown for the following considered cases: 3D (solid line), 2D (dash–dot line), Gaussian Q2D ($a = 75$ Å) without summation over the intermediate states (dashed line), and Gaussian Q2D ($a = 75$ Å) with summation over all the intermediate states (dotted line). As can be seen, the curves obtained by taking into account the contributions of all the intermediate states are between the 2D and the corresponding 3D curves with an effect which assures the correctness of the self-energy. We plotted in figure 7 the cyclotron resonance frequency corresponding to the lower magneto-polaron branches shown in figure 6. Thus, we can observe that the effect of the summation over all the intermediate states, as far as cyclotron resonance is concerned, is of minor importance.

By systematically taking into account all the sources of the system's anisotropy, we presented here the effects of the anisotropy and the finite z-extent of the electron wavefunction on the magneto-polaron spectrum in a geometry with magnetic field directed along the optical axis. In particular the anisotropic properties of the extraordinary-phonon spectrum are found to be very important, imposing new features on the distribution of the cyclotron resonance frequencies as follows:

(i) the presence of quasi-transverse phonons assures, from below, the pinning of the lower cyclotron resonance frequency branch to the lowest phonon frequency $\omega_{TO}^{\perp}$ (in this particular case of InSe) at very large magnetic field;
(ii) the cyclotron resonance frequency of the upper magneto-polaron branch is situated above the highest phonon frequency $\omega_{LO}^{\perp}$ independently of the strength of the electron–phonon-interaction;

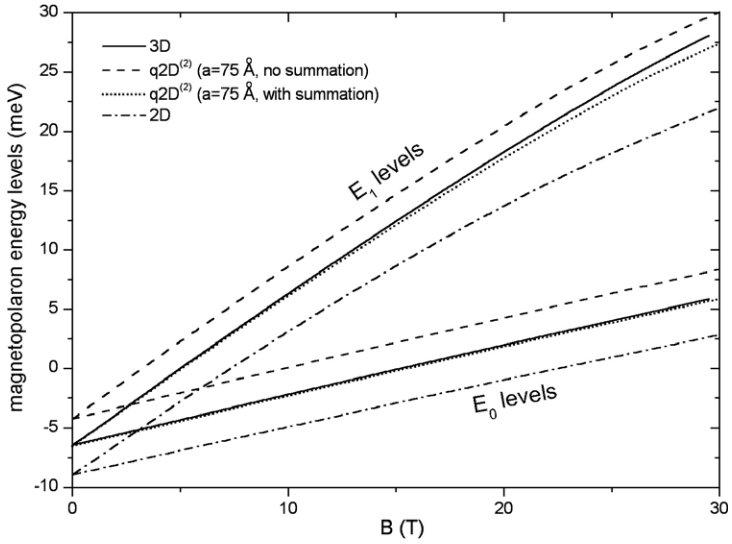

Figure 6. The first two Landau levels for the Q2D InSe magneto-polaron energy spectrum calculated using the second trial electron wavefunction (Gauss function) with (dotted line) and without (dashed line) summation over the intermediate states. The 3D (solid line) and 2D (dash–dot line) cases are also shown.

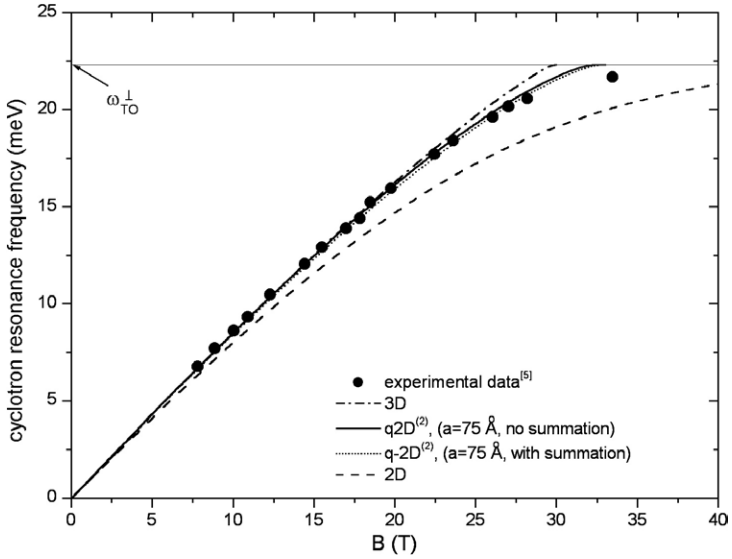

Figure 7. The lower cyclotron resonance frequency branch for Q2D InSe calculated using the second trial electron wavefunction (Gauss function) with (dotted line) and without (solid line) summation over the intermediate states. For comparison, the 3D (dash–dot line) and 2D (dashed line) results are shown.

(iii) there is a new branch of the cyclotron resonance frequency situated in the phonon frequency domain ($\omega_{\mathrm{TO}}^{\parallel}$, $\omega_{\mathrm{LO}}^{\parallel}$).

A generalization to the case of a material having a richer infrared reflectivity/absorption spectrum is possible.

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