The lower magnetopolaron branch contribution to the cyclotron resonance in layer compound InSe

D.E.N. Brancus [a,1], G. Stan [b], A. Dafinei [a]

[a] *Faculty of Physics, University of Bucharest, P.O. Box MG-11, Bucharest, Romania*

[b] *Department of Physics, Colorado State University, Fort Collins, Colorado, 80523, USA*

Abstract

The energy of a weak-coupling Fröhlich polaron in a uniaxial anisotropic semiconductor with complex structure, placed in a d.c. magnetic field directed along the optical axis, are obtained in the context of the improved Wigner-Brillouin perturbation theory. We consider a quasi-two-dimesional (q-2D) behavior of the conduction electron whereas the phonon sysytem is a three-dimensional one. In order to avoid the real phonon emission phenomenon, the discussion is restricted to the lower branch of the magnetopolaron spectrum. The contributions of all sources of anisotropy to the magnetopolaron spectrum are sistematically considered. The q-2D behavior of the electron gas is taken into account by considering a finite extent along the optical axis of a variational electron wave function. In the particular case of parabolic form for the confining potential, the theoretical results could be improved by considering the contribution of all intermediate states to the cyclotron resonance phenomenon.

Key words: magnetopolaron; cyclotron resonance; anisotropic layer compounds.

The measurements of Subnikov- de Hass oscillations and cyclotron resonance performed at low temperatures in the layered compound InSe [1], have shown an apparently two-dimensional (2D) behavior of the electron gas. The extension [2] of the cyclotron measurements in the domain of magnetopolaron splitting argued for considering a finite width of the electron gas. However, in the spite of its succes in the explanation of the experimental results, the model used in Ref.2 discusses the effect of the sources of anisotropy on the cyclotron resonance in a simplified manner. In this paper the results obtained [3] for the energy spectrum of an anisotropic (uniaxial) 3D polaron in a magnetic field are extended to the q-2D case by coherently taking into account the contributions of all sources of anisotropy.

In the presence of both a magnetic field $\mathbf{B}_0$ (introduced by a symmetrical Coulomb gauge) directed along the optical axis (parallel with z-axis) and a confining potential $V(z)$, the Hamiltonian of a conduction electron interacting with optical phonons in a uniaxial polar crystal having a complex structure is:

$$H = \hbar\omega(A^+A + 1/2) + \frac{p_z^2}{2m_\parallel} + V(z)$$
$$+ \sum_{\mathbf{q},\mu} \hbar\omega_\mu(\mathbf{q}) b^\dagger_{\mathbf{q},\mu} b_{\mathbf{q},\mu} + \sum_{\mathbf{q},\mu} (\frac{V_\mu(\mathbf{q})}{\sqrt{V}} b_{\mathbf{q},\mu} e^{i\mathbf{q}\cdot\mathbf{r}} + H.c), \quad (1)$$

where, the significance of the involved quantities is given in Ref.3.

In the frame of Wigner-Brillouin perturbation theory, 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 expression (see Ref.4 for some details):

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

[1] dane@solid.fizica.unibuc.ro

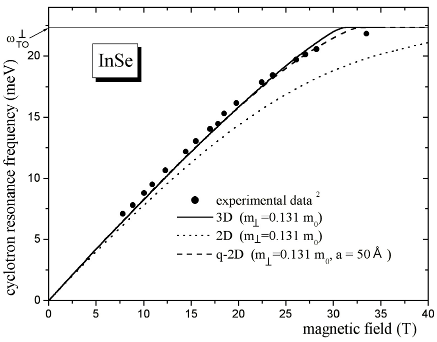

Fig. 1. The lower magnetopolaron branch in InSe considering a 3D (continuous line), 2D (dot line), and q-2D Fang-Howard (dash line) electron wave function, respectively. The calculation was done using $m_\perp = 0.131 m_0$ and $m_\parallel = 0.081 m_0$ for the bare electron effective mass tensor.

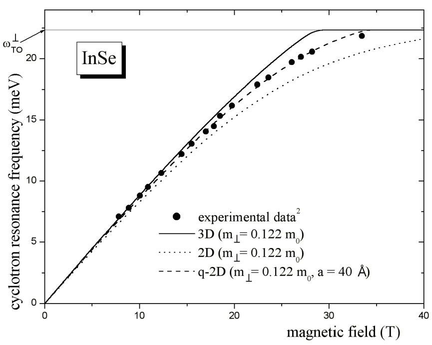

Fig. 2. The lower magnetopolaron branch in InSe considering a 3D (continuous line), 2D (dot line), and q-2D gauss (dash line) electron wave function, respectively. The calculation was done using $m_\perp = 0.122 m_0$ and $m_\parallel = 0.081 m_0$ for the bare electron effective mass tensor. The summation over the intermediate states was included.

where $|l\rangle$ and E_l denote the state and, respectively, the energy of the eigenvalue problem corresponding to the electron z-motion.

Working at zero temperature and considering that the energies of the excited states for z-motion are larger than those in the (x,y) plane, we could restrict ourselves only to the contribution of the fundamental state $|l_0\rangle$. The finite z-extent of the electron wave function in the symmetrical planar layer is considered by taking into account two forms for the wave function: the one verifies $|\varphi_{l_0}^{(1)}(z)|^2 = (2a)^{-1} e^{-|z|/a}$ (also considered in Ref.2) and the other is a Fang-Howard function type, $\varphi_{l_0}^{(2)}(z) = (2a^{3/2})^{-1} z e^{-|z|/2a}$.

Fig.1 shows the magnetic field dependence of the cyclotron resonance frequency in InSe for the considered cases (3D, q-2D, and 2D), calculated for the first form of the variational electron wave function. The cyclotron resonance energy is defined as the difference between the first two perturbed Landau levels.

We can observe that, excepting the last experimental point, in the domain of large magnetic fields the experimental results are quite well fitted with the first variational wave function for the value $a = 50\mathring{A}$. Similar results are obtained (but for $a = 20\mathring{A}$) for the second form of the electron wave function. Though the two values of the parameter "a" which realize the best fitting are different, the width of the q-2D electron layer defined as $w = \langle (z - \langle z \rangle)^2 \rangle^{1/2}$ has the same value ($a = 70\mathring{A}$) for both electron wave functions. Therefore, the results seem to be independent of the concrete form of the variational wave function. We have to stress that, in contradistinction with the model developed in Ref.2, we do not use, excepting "a", other fiting parameters.

In the following we will give some corrections to the above formulation of the problem. It is clear that restricting us only to the contribution of the fundamental state $|l_0\rangle$, the 3D limit of the problem ($a \to \infty$) cannot be obtained. In addition, based on an estimation of the electron binding energies [5] of an order of $20-30 meV$, we conclude that, at least for high magnetic field values, the above considered restriction could be amended. In order to take into consideration the contributions of all intermediate states $|l\rangle$, we parameterized the confining potential by a parabolic form, i.e. a Gaussian expression $\varphi_0(z) = \pi^{-1/4} a^{-1/2} e^{-z^2/2a^2}$ for the wave function of the fundamental state. At least at low temperature, this assumption is quite resonable. Also, we consider the effective mass component $m_\perp$ of the bare electron as a second fitting parameter. These results are presented in Fig.2 which shows a very good fitting of the experimental point distribution for the q-2D curve with $a = 40\mathring{A}$. All the curves are obtained for $m_\perp = 0.122 m_0$. With this new value for $m_\perp$ the width of the electron gas layer is different from that obtained before. Therefore, instead to consider the anisotropic electron-phonon coupling constants as fitting parameters (as it was done in Ref.2), the most natural way is realized by taking the components of the effective mass tensor of the bare electron as having this character. However, to find the values of the components of the effective mass tensor for the bare electron the developed procedure has to assure the best fitting also for the upper magnetopolaron branch contribution.

References

[1] J.C. Portal et al., J. Phys. Soc. Japan. Suppl. **A 49**,(1980) 879.

[2] R.J. Nicholas et al., Phys. Rev. **B 45**, (1992) 12144.

[3] D.E.N. Brancus, G. Stan, Phys. Rev. **B 63**, 235203 (2001).

[4] F.M. Peeters, J.T. Devreese, Phys. Rev. **B 31**, 3689 (1985).

[5] E. Kress-Rogers, R.J. Nicholas, J.C. Portal, A. Chevy, Solid State Commun. **44**, 379 (1982).