Cyclotron Resonance of Interface Polarons in Semiconductor Heterostructures

Francisco A.P. Osório
Departamento de Física, Instituto de Matemática e Física
Universidade Federal de Goiás, C.P. 131, 74001-970, Goiânia, Goiás, Brasil

Marcos H. Degani and Oscar Hipólito
Departamento de Física e Ciências dos Materiais, Instituto de Física e Química de São Carlos
Universidade de São Paulo, C.P. 369, 13560-970, São Carlos, SP., Brasil

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Corrections to the cyclotron resonance energy and electron effective mass due to electron-interface LO-phonon modes interaction in semiconductor heterostructures, are calculated as a.function of the magnetic field perpendicular to the surface through tlie second order of the Improved Wigner-Brillouin Perturbation Theory (IWBPT). The Fröhlich model describing this system is employed throughout. Numerical results for GaAs-GaSb and GaAs-AlAs heterojunctions are obtained and shown important contribution due to tlie interface modes on near the resonance region. In the case where the interface mode is close to the bulk mode a three branches splitting appear in the cyclotron energy and effective mass. We also have found that the resonance frequencies are shifted frorn its original positions due to tlie presence of other modes. Foi GaAs-AlAs heterostructures in the region below the resonance where the experiments are usualy carried out tlie electron interaction with the iiiterface phonons can be neglected. The inclusion of tlie bulk phonons of GaAs only give good enough results. It is suggested that experiments should be carry out to confirm our results.

I. Introduction

In the last few years has been highly increased tlie interest in the polaronic effects on tlie properties of quasi-two-dimensional clcctrons systems confined in polar semiconductor heterostructures. The majority of the theoretical works about this subject consider only the interaction of tlie electron with the longitudinal optical (LO) phonons or the material bulk, not taking into account the interaction with the interface optical (IO) phonons. But as it was shown by some authors[1,2,3] in some situation tlie electron-interface phonon coupling is very important and not can be neglected.

As suggested[4] one of such a situation cnii be founcl in Cyclotron Resonance (CR) experiments, where tlie electron-phonon resonant coupling give rise to a discontinuity in the effective mass. However in CR experiments realized, the most for the GaAs-AlGaAs heterostructures, tlie effect of the electron-IO phonon interaction was not observed. But the interfacial inodes were observed in superllatices of GaAs-AlGaAs by Sood, et al[5] in backscattering Raman spectra, by Lambin et al[6] in high-resolution electron-energy loss spectra, and by Meynadier ct al[7] in Raman scattering of high-order a.t the resonance with the lowest optical transition.

Recently some theoretical works[8,9,10] on CR of polarons in heterostructures that consider the electron LO- and IO-phonon interactions, have been appeared. However in these works the treatment given to the interfacial modes is incomplete and not satisfactory. For a.polar semiconductor heterojunction, discontinuities in

the cyclotron mass occur in IO and LO phonon frequencies. When tlie interfacial mode frequency is isolated of the other frequencies the resonant splitting of the cyclotron mass occurs is ill two branches. If the frequeiicy of two modes are close, the resonant splitting can occur in three branches[9].

The purpose of the present work is to study the effects of electron IO- and LO-phonon interactions oii the electron cyclotron mass in a semiconductor heterojunction of polar materials, giving a correct treatment[11] to the interfacial modes. We use the improved Wigner-Brillouin perturbation theory (IWBPT) to calculate the polaronic correction to the Landau levels, not including in the calculation tlie screening of the electron-phonon interaction and the nonparabolicity of the conduction band. Such effects are very important to precise determination of cyclotron mass, but since the experimental results are not available until now it were ignored. Its inclusion not change tlie positions of the resonant points.

II. Polaronic correction to the Landau levels

Let us consider a heterojunction composed of two semi-infinite polar semiconductors, with interface placed at $z = 0$. The material 1 occupying the region $z > 0$ and the material 2 the region $z < 0$. Each medium is characterized by the dielectric function,

$$\epsilon_n(\omega) = \epsilon_{\infty_n} \frac{(\omega_{Ln}^2 - \omega^2)}{(\omega_{Tn}^2 - \omega^2)} \tag{1}$$

where ω_{Ln} (ω_{Tn}) is the LO (TO) phonon frequency of material n (n=1,2) with optical dielectric constant ϵ_{∞_n} and static clielectric constant ϵ_{O_n}. To this system a uniform magnetic field $\vec{B}$ in tlie z direction, perpendicular to interface, is apllied.

The Hamiltonian of one electron in the conduction band of material 1, interacting with the LO and IO phonons can be written as,

$$H = H_0 + H_1, \tag{2}$$

where H_0 is tlie Hamiltonian of one electron under tlie action of a uniform magnetic field plus the Hamiltonian of a free-phonon system,

$$H_0 = \frac{1}{2m_b}\left(\vec{P} - \frac{e}{c}\vec{A}\right)^2 + V(z) + \sum_{\vec{Q}} \hbar\omega_{L1} a_{\vec{Q}}^{+} a_{\vec{Q}} + \sum_{j=1}^{2}\sum_{\vec{Q}} \hbar\omega_{Ij} b_{\vec{Q}_j}^{+} b_{\vec{Q}_j} \tag{3}$$

where $V(z)$ is the confining potential of the electron with momentum operator $\vec{P}$, coordinates $\vec{r} = (\vec{\rho}, z)$ and band mass m_b. The energy and tlie wave vector of bulk LO plionoii in material 1, are $\hbar\omega_{L1}$ and $\vec{Q} = (\vec{q}, q_z)$ respectively, and $a_{\vec{Q}}^{+}(a_{\vec{Q}})$ is tlie creation (annihilation) operator. ω_{Ij} is tlie interface optical phonon frequency tliat satisfies the dispersion relation $\epsilon_1(\omega_{Ij}) + \epsilon_2(\omega_{Ij}) = 0$, mhere the indices $j = 1$ and $j = 2$ denote $\omega_{I1} = \omega_-$ and $\omega_{I2} = \omega_+$, the two modes of IO phonons, with creation (annihilation) opcrator $b_{\vec{Q}_j}^{+}(b_{\vec{Q}_j})$. $\vec{A}$ is the magnetic vector potential assumed in the Landau gauge.

Tlie electron-LO and-IO phonon interactions are given by H_1,

$$H_1 = H_{e-LO} + H_{e-IO} \tag{4}$$

mhere,

$$H_{e-LO} = \sum_{\vec{Q}} \left[V_{\vec{Q}} e^{i\vec{q}\cdot\vec{\rho}} \sin(q_z z) a_{\vec{Q}} + h.c\right] \tag{5}$$

and

The Fourier coefficients for tlie interaction described in the above equations are,

$$V_Q = -\frac{i}{Q}\left(\frac{4\pi e^2}{V}\left(\frac{1}{\epsilon_{\infty 1}} - \frac{1}{\epsilon_{01}}\right)\hbar\omega_{L1}\right)^{1/2} \quad (7)$$

and

$$\Gamma_q = -\frac{i\hbar\omega_{Ij}}{\sqrt{q}}\left(\frac{2\pi}{S}\alpha_j r_{p_j}\right)^{1/2} \quad (8)$$

respectively, wliere V is tlie volume and S the area of system. $r_{p_j} = (\hbar/2m_b\omega_{Ij})^{1/2}$is the interface polaron radius and α_j the electron-IO phonon coupling constant, defined as.

$$\alpha_j = \left(\frac{e^2}{\hbar\omega_{Ij} r_{p_j}}\right)\left\{\frac{\omega_{Ij}^2}{\omega_{p1}^2}\left(\epsilon_1(\omega_{Ij}) - 1\right)^2 \Theta_1(\omega_{Ij}) + \frac{\omega_{Ij}^2}{\omega_{p2}^2}\left(\epsilon_2(\omega_{Ij}) - 1\right)^2 \Theta_2(\omega_{Ij})\right\}^{-1} \quad (9)$$

The ion plasma frequency, ω_{pn}, and the fuiictioii O, (w) are given by

$$\omega_{pn}^2 = \left(9\epsilon_{\infty n}\frac{(\omega_{Ln}^2 + \omega_{Tn}^2)}{(\epsilon_{\infty 2} + 2)^2}\right) \quad (10)$$

and

$$\Theta_n(\omega) = \left(1 + \frac{\epsilon_{On}}{3\epsilon_{\infty n}}\frac{(\epsilon_{\infty n} - 1)(\epsilon_{\infty n} + 2)}{(\epsilon_{0n} - \epsilon_{\infty n})\omega_{Ln}^2}(\omega_{0n}^2 - \omega^2)\right)^{-2} \quad (11)$$

with

$$\omega_{0n}^2 = \left(\omega_{Ln}^2 - \frac{2(\omega_{Ln}^2 - \omega_{Tn}^2)}{\epsilon_{\infty n} + 2}\right) . \quad (12)$$

The electron-optical (LO and IO)-phonon interaction shifted tlie energy of tlie Landau levels by a quantitity ΔE_N,

$$E_N^* = (N + \frac{1}{2})\hbar\omega_c + \Delta E_N , \quad (13)$$

which in the weak coupling regime, can be calculated by the second-order perturbation theory. The correct one to the polaron problem, is the improved Wigner-Brillouin perturbation theory, IWBPT, which gives tlie correct pinning behavior. In such a way we have,

$$\Delta E_N = -\sum_{\vec{Q}}\sum_{j}\sum_{N'=0}^{\infty}\frac{|< \Psi_{N\,ky} - q_y|H_1|\Psi_{N\,ky} > |^2}{\hbar\omega_j - (N - N')\hbar\omega_c - \Delta_N} \quad (14)$$

where tlie sum over j involve all tlie three phonons modes with frequencies $\hbar\omega_j$, and $\omega_c = (eB/m_b)$ is the cyclotron resonance frequency. The value of energy shift Δ_N, in the IWBPT, is given by, $\Delta_N = \Delta E_N - \Delta E_o$, wliere AE, is calculated by the Rayleigh-Schrödinger perturbation theory (RSPT), and

$$|\Psi_{N,ky} >= |N, k_y; 0_{\vec{Q}}; 0_{\vec{q}} > \quad (15)$$

is the ivave function of tlie non perturbed Hamiltonian, H_0. $|N >= u_N(x - k_y l^2)$ is the harmonic oscilator wave function with a. displaced center, $l^2 = \hbar/eB$ being the radius of the classical cyclotron orbit. $|0 >_{LO}$ and $|0 >_{IO}$ denote the vacuum of L 0 and 10 phonons, $|k_y >= e^{ik_y y}$ is tlie electron wave function in the y direction and $\xi(z)$ is the Fang-Howard variational wave function for tlie motion perpendicular to the interface, which is $\xi(z) = (b^3/2)^{1/2} z e^{-bz/2}$ for $z \geq 0$, and $\xi(z) = 0$ for $z < 0$. The parameter b is obtained by minimizing tlie energy of tlie system, and is given as

$$b^3 = \left(\frac{48\pi m_b e^2}{\epsilon_{01}\hbar}(N_d + \frac{11}{32}N_s)\right) \quad (16)$$

wliere N_d and N_s are tlie depletion and electron density respectively. By introclucing in the equation (14) the Hamiltonian H_1, the wave function, converting the sum over the phonons wave vector into integrals and realizing the integral over the z-component, we obta:

$$\Delta E_N = -\alpha \int_0^\infty du F_H(u) \sum_{N'=0}^{\infty} \frac{|V_{NN'}(u)|^2}{1-(N-N')\lambda^2 - \Delta_N} + \\ -\sum_{j=1}^{2} \alpha_j \left(\frac{\hbar\omega_{Ij}}{\hbar\omega_{L1}}\right) \int_0^\infty du_j F_I(u_j) \sum_{N'=0}^{\infty} \frac{|V_{NN'}(u_j)|^2}{1-(N-N')\lambda_{Ij}^2 - \Delta_N(\frac{\lambda_{ij}^2}{\lambda^2})}, \quad (17)$$

where all the lengths and energy are taken in units of polaron radius $r_p = (\hbar/2m_b\omega_{L1})^{1/2}$ and energy $(\hbar\omega_{L1})$. We are using the following dimensionless parameters: $\lambda^2 = \hbar\omega_c/\hbar\omega_{L1}, \lambda_j^2 = \hbar\omega_c/\hbar\omega_{Ij}, u = qr_p$ and $u_j = qr_{pj}$. The matrix element of the electron-phonon interaction operator. $V_{NN}^{'}(q)$, can be written as,

$$|V_{NN'}(q)|^2 = \frac{n_2!}{n_1!}\exp\left(-\frac{q^2\ell^2}{2}\right)\left(\frac{q^2\ell^2}{2}\right)^{n_1-n_2}\{L_{n_2}^{n_1-n_2}(q^2\ell^2/2)\}^2, \quad (18)$$

where $n_2 = min(N,N')$, $n_1 = max(N,N')$ and $L_n^k(x)$ is the associated Laguerre polynominal. The form factor $F_H(q)$ is defined as,

$$F_H = \int_0^\infty dz \int_0^\infty dz' |\xi(z)|^2|\xi(z')|^2(e^{-q|z-z'|} - e^{-|z+z'|}) = F(q) - F_I(q), \quad (19)$$

and,

$$F(q) = \int_0^\infty dz \int_0^\infty dz' |\xi(z')|^2 e^{-q|z-z'|}, \quad (20)$$

is the quasi-two-dimensional (Q2D) form factor, and $F_I(q)$, is the interface form factor

$$F_I(q) = \int_0^\infty dz \int_0^\infty dz' |\xi(z)|^2|\xi(z')|^2 e^{-|z+z'|} = \frac{b^6}{(b+q)^6}. \quad (21)$$

It is interesting to note that we recover here the quasi-two-dimensional case, where the electron interacts with the bulk LO phonons only, via the usual Fröhlich hamiltonian, by taking $F_I = 0$. in the above equations.

The polaron cyclotron mass is determined through the cyclotron resonance frequency $\omega_c^* = (eB/m^*)$, that is defincd as the diference between the two first perturbed Landau levels $N = 0$ and $N = 1, \hbar\omega_c^* = E_1^* - E_0^*$,

$$m^* = m_b\left\{1 + \frac{\Delta E_1 - \Delta E_0}{\lambda^2}\right\}^{-1} \quad (22)$$

where ΔE_1 and ΔE_0 are obtained of the numerically evaluation of the equation (17).

III. Results

Our numerical results are for heterojunctions of GaAs-GaSb and GaAs-AlAs. All ofthe calculations assume that the electrons are placed in the GaAs, material l. The electronic density considered is $N_s = 10^{11}cm^{-2}$, which is an usual density in the experimental situation and $N_d = 0$. The physical parameters of the materials used here are listed in the Table I. The electron-IO phonon coupling constants and IO phonon frequencies are:$\omega_{I1} = 238.08cm^{-1}, \alpha_1 = 0.034; \omega_{I2} = 281.13cm^{-1}$ and $\alpha_2 = 0.019$ to GaSb-GaAs heterojunction; and $\omega_{I1} = 283.24cm^{-1}; \alpha_1 = 0.029; \omega_{I2} = 382.33cm^{-1}$ and $\alpha_2 = 0.053$ for $AlAs - GaAs$ heterojunction. The $GaAs$ electron-LO phonon coupling constant, is assumed to be $\alpha = 0.068$.

Table I: The characteristics parameters of the materials used in the numerical calculations.

	ϵ_0	ϵ_∞	$\omega_{Ln}(cm^{-1})$	$\omega_{Tn}(cm^{-1})$
GaAs	12.83	10.90	295.80	272.64
GaSb	15.69	14.44	240.19	230.42
AlAs	10.20	81.60	404.03	361.29

For $GaSb-GaAs$ heterojunction the interface mode frequency ω_{I1} is much smaller then the other two modes ω_{I2} and ω_{L1}. Then in the resonance, $\omega_c = \omega_{I1}$, the contribution to $\Delta E_1(N' = 0)$ from these modes can be neglected and the splitting of the cyclotron mass occiirs ill two branches as it is shown in Fig. 1, where the mass is plotted as a. function of magnetic field through the parameter $\lambda^2 = \hbar\omega_c/\hbar\omega_{L1}$. The dashed curve denotes the case where the electron-IO phonon interaction is not taken into account. Tlie first split in this Figure appears a.t $\lambda^2 \cong 0.83$ instead of 0.805 as expected for $\omega_c = \omega_{I1}$. Tlie same shift but smaller also occurs in tlic next split around $\omega_c = \omega_{I2} \cong \omega_{L1}$ at $\lambda^2 \sim 0.96$. In this case both modes contribute to ΔE_1 and the split of the mass occurs in three branches. A better calculation to this tri-split region should be made in a more rigorous way such as done by Larsen[12] in the case of confined polarons. Here we are restricted to an approximation of Eq.(17) with $N' = 0$. As we see from Fig. 2 an extra branch appears between the well known other two branches.

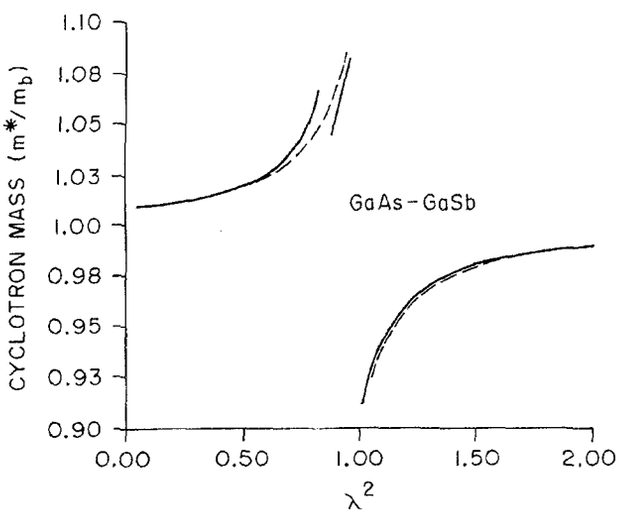

Figure 1: Cyclotron mass as a function of external magnetic field through the dimensionless parameter $\lambda^2 = \omega_c/\omega_{L1}$ for $GaAs - GaSb$ heterojunction with electronic density $N_S = 10^{11} cm^{-2}$ and $N_d = 0$. The solid curves are tlie results by including the interface phonons in the calculation. The dashed curves are the results with the presence of tlic bulk LO phonons only.

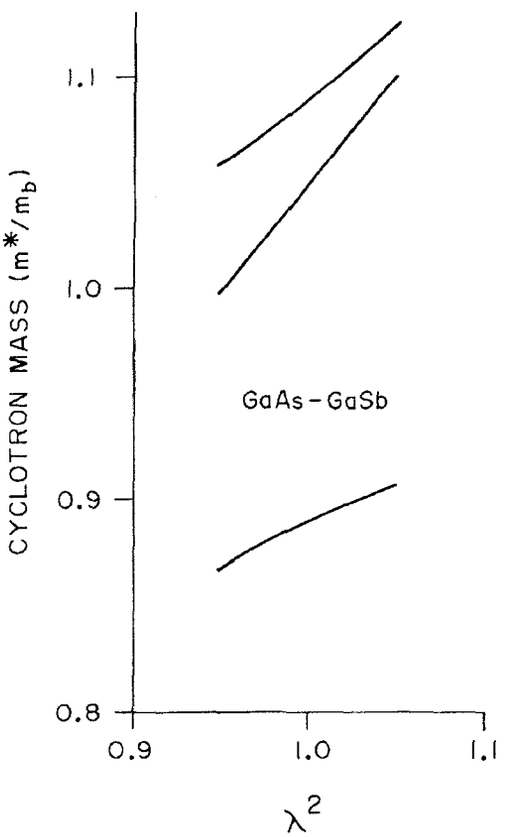

Figure 2: The tri-split resonance branches of the polaron cyclotron mass presents in the $GaAs - GaSb$ heterojunction.

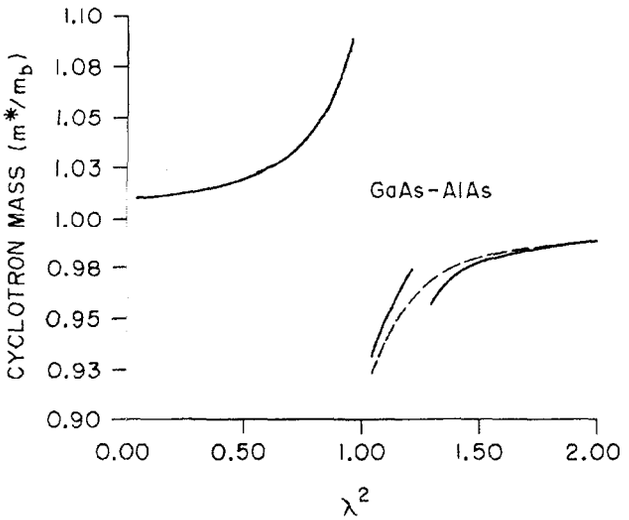

Figure 3: The same as Figure 1 for $GaAs - AlAs$ heterojunction.

In Fig. 3 we shown the cyclotron mass for $GaAs - AlAs$ heterojuilction. The overall behavior is similar to that of the previous system. The difference is that here the interface frquency ω_{I2} is much larger than the other

two modes ω_{I1} and ω_{L1}. Then for large magnetic field $\omega_c > \omega_{L1}$ there is a mass discontinuity at $\gamma^2 \simeq 1.2$ due to the electron-interface phonon interaction instead of $\lambda^2 = 1.293$ as expected for tlie ω_{I2} frequency. In this case the resonance is shifted to left in contrast to the GaSb system. We also note that the contribution of the interface phonon is quite important for large values of tlie magnetic field.

In conclusion, from our results the presence of interface phonons play a fundamental role in the understanding of the polaron cyclotron mass mainly in the region near the resonance. In the case of $GaAs-AlAs$, for low magnetic field, where tlie experiments are carried on it is enough to consider the presence of bulk LO phonon only, in the calculations. But to precisely determine tlie resonances it is necessary to take into account tlie presence of interface phonons.

The shifts on the resonance frequencies are due to the contribution of other modes and to the best of our knowledgement were not experimentally observed yet.

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