Crossing of spin energy sublevels in InSb-based stepped quantum wells under in-plane magnetic field: Intersubband optical absorption.

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We study the energy dispersion relations for InSb-based stepped quantum wells when Zeeman splitting is present. Spin level crossing can be achieved by applying certain pairs of transverse electric and in-plane magnetic field values. We use an improved $4 \times 4$ version of the Transfer Matrix Approach which, together with first order boundary conditions, leads to a momentum dependent pseudo Wronskyan matrix. Roots of this matrix give the dispersion relations showing spin level crossings and anticrossings. In order to analyze the effects of spin crossing we calculate linear and non-linear absorption coefficients for transitions between the four deepest sublevels after Zeeman splitting. We also consider depolarization shift caused by different charge concentrations. Results show a noticeable difference on the structure of the intersubband absorption spectrum when spin sublevel crossing is present.

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I. INTRODUCTION

It is well-known that the key of spintronics is the breakdown of the degenerate electronic levels by the spin splitting [1]. This means that spin up and spin down electronic (hole) states of any material must necessarily be separated in energy. One way of achieving this splitting is to use two-dimensional electron gas (2DEG) in quantum wells (QWs). In semiconductor QWs this effect is obtained spontaneously, without external magnetic fields, as long as the confining potential is not symmetrical. Spin splitting will increase due to the contribution of the Zeeman effect when an external in-plane magnetic field is applied [2, 3].

Some semiconductors are particularly suitable materials for spintronics. One of them is the InSb with a large Landé factor, which causes a big magnetic energy and the consequent Zeeman splitting. Also, materials with narrow gap are appropriate for spintronic, and InSb has a narrow gap. We have chosen in this study this material by the two mentioned reasons.

Non symmetric heterostructures under in-plane magnetic field show non parabolic dispersion relations. For each electronic level, non parabolic spin splitted subbands with opposite spin are shifted by the magnetic field in opposite directions of the momentum space. This behavior leads to the presence of anticrossings between subbands for certain momentum values, which are reflected in some peculiarities of the joint density of states and in the excitation photoluminescence spectrum [4–6].

For particular structures with two close electronic levels, high enough magnetic fields can cause a Zeeman splitting of each level bigger than the interlevel energy distance. In this case, together with the momentum-space displacements for different spin sublevels, we have different curvature of quasi parabolas for different electronic levels leading to crossings between the two distinct electronic levels with opposite spins. We should note that, now, we are not talking about anticrossings but crossings, which has been less studied [7–9].

To obtain close enough energy levels, with an intersubband energy distance of the order of the spin splitting, we propose an InSb-based stepped QW.

The standard way to study the optical properties of a material is through electronic transitions that occur after exposing the sample to a perturbation, usually photoexcitation. From a theoretical point of view this means a precise knowledge of the band structure and, hence, the dispersion relations. Several methods were used to calculate the dispersion relations in quantum structures. Among them, the Transfer Matrix Approximation (TMA),
together with first order boundary conditions \[10\], is particularly suitable for low-symmetry structures because of its versatility. Moreover, this method allows us to add a wide range of perturbations as transverse electric and in-plane magnetic fields. Another effect we can add is abrupt barrier contribution for narrow gap structures.

Optical absorption is one of the most used experimental techniques to study band structures. Absorption spectrum strongly depends on the electronic concentration when heterostructure is selectively doped. Essentially, electronic density is reflected in a variation of the frequency transition between subbands.

The purpose of this work is the study of peculiarities of intersubband optical absorption produced by the crossover of spin sublevels, including electronic concentration effects.

II. THEORETICAL FRAMEWORK

A. Eigenstates

In the parabolic approximation, the one-electron Schrödinger equation for stepped QW can be written as \[6, 11\]:

\[
\left( \varepsilon^\mu(p) + \frac{p^2}{2m^\mu} + U^\mu(z) + \hat{W}^\mu(p) \right) \Psi^\mu(p,z) = E \Psi^\mu(p,z),
\]

for each 2D momentum \( p = (p_x, p_y) \), where \( \Psi^\mu(p,z) \) and \( E \), are the eigenfunctions and eigenvalues, respectively. Superscript \( \mu = b, w_1, w_2 \) means barrier or wells (wide and narrow), respectively. The kinetic energy in the in-plane direction, \( \varepsilon^\mu(p) \), includes the effective mass \( m^\mu \).

The potential energy \( U^\mu(z) \) is \( U^\mu(z) \simeq U^\mu_0 + eF_\perp z \) with \( U^\mu_0 = \Delta E_{c2b} \) in the barriers, \( U^w_1 = \Delta E_{c12} \) in the wide well, and \( U^w_2 = 0 \) in the narrow well. \( F_\perp \) is an uniform transverse electric field, and the band offsets for conduction band are \( \Delta E_{c12} \) between both wells, and \( \Delta E_{c2b} \) between \( w_2 \) and barrier. Band diagram for the stepped QW is shown in Fig. 1.

For not very strong magnetic fields, we describe the magnetic energy as \( \hat{W}^\mu = \overline{\nabla^\mu} [\hat{\sigma} \times p]_z + w^\mu_H \hat{\sigma}_y \), where \( \hat{\sigma} \) is the Pauli matrix, and \( w^\mu_H = (\overline{\gamma}^\mu/2)\mu_B H \) is the Zeeman splitting caused by the magnetic field. Here \( \overline{\gamma}^\mu \) is the effective Landé factor, \( \mu_B \) is the Bohr magneton, and \( H \) is the in-plane magnetic field. Due to the different effective masses, characteristic spin velocity for each layer is \( \overline{\gamma}^\mu = eF_\perp \hbar/4m^\mu \varepsilon_g^\mu \), with \( \varepsilon_g^\mu \) the gap energy.
After some heavy algebra [12], we obtain the fundamental solutions of Eq (1) for spin \( \sigma = (\uparrow, \downarrow) \):

\[
\Psi^{\mu \uparrow}(p, z) = \left\{ a_{\mu \uparrow} + b_{\mu \uparrow} B(i\xi_{\mu \uparrow}) \right\} + \\
+ \rho^{\mu \uparrow}(p) \left\{ a_{\mu \uparrow} Ai(\xi_{\mu \uparrow}) + b_{\mu \uparrow} Bi(\xi_{\mu \uparrow}) \right\} \left(1/\sqrt{2}\right)
\]

\[
\Psi^{\mu \downarrow}(p, z) = \left\{ \rho^{\mu \downarrow}(p) \left\{ a_{\mu \downarrow} Ai(\xi_{\mu \downarrow}) + b_{\mu \downarrow} Bi(\xi_{\mu \downarrow}) \right\} + \\
+ \left[ a_{\mu \downarrow} Ai(\xi_{\mu \downarrow}) + b_{\mu \downarrow} Bi(\xi_{\mu \downarrow}) \right] \right\} \left(1/\sqrt{2}\right),
\]

(2)

where \( \rho^{\mu \pm}(p) = (\bar{v}_{\mu} p_{\pm} + \bar{w}_{\mu})/iw_{\mu}(p) \), with \( p_{\pm} = p_{x} \pm ip_{y} \) and \( w_{\mu}(p) = [(\bar{v}_{\mu} p_{x} + \bar{w}_{\mu})^2 + (\bar{v}_{\mu} p_{y})^2]^{1/2}. \) In the above equation \( Ai(\xi_{p}^{\mu \sigma}) \) and \( Bi(\xi_{p}^{\mu \sigma}) \) are the Airy functions with arguments

\[
\xi_{p}^{\mu \sigma} = \frac{z}{l_{\perp}} + \frac{\varepsilon_{\mu}^{\sigma}(p) - E + U_{0}^{\mu}}{\varepsilon_{\perp}^{\mu}}.
\]

(3)

with the following auxiliary parameters: the length \( l_{\perp} = (\hbar^2/2m_{\mu}eF_{\perp})^{1/3} \), and energies \( \varepsilon_{\perp}^{\mu} = \hbar^2/[2m_{\mu} (l_{\perp}^2)], \varepsilon_{\mu}^{\uparrow}(p) = \varepsilon_{\mu}^{\downarrow}(p) + |w_{\mu}(p)|, \) and \( \varepsilon_{\mu}^{\downarrow}(p) = \varepsilon_{\mu}(p) - |w_{\mu}(p)|. \) Lastly, \( a_{\mu \sigma}, b_{\mu \sigma} \) are unknown coefficients that we will obtain by means of the boundary conditions, including abrupt interface parameter [13] \( \chi^{\mu \nu} = (2eF_{\perp} \delta + \left|U_{0}^{\mu} - U_{0}^{\nu}\right|)/2\varepsilon_{\nu}^{\nu} \approx \left|U_{0}^{\mu} - U_{0}^{\nu}\right|/2\varepsilon_{\nu}^{\nu}, \) where \( \delta \) is the halfwidth of that interface [12].

The following step is to generate \( 4 \times 4 \) Wronskian-like transfer matrices, \( M^{\mu}(L_{i}, E, p) \), which involve contour conditions at interface \( L_{i}. \) To obtain electronic levels for each 2D momentum \( p = (p_{x}, p_{y}) \) we introduce a modification of the method used before [12]. The total transfer matrix can be written as:

\[
S(E, p) = \left[M^{b}(L_{1}, E, p)\right]^{-1} \cdot M^{w_{1}}(L_{1}, E, p) \cdot \\
\left[M^{w_{2}}(L_{2}, E, p)\right]^{-1} \cdot M^{w_{2}}(L_{2}, E, p) \cdot \\
\left[M^{w_{2}}(L_{3}, E, p)\right]^{-1} \cdot M^{b}(L_{3}, E, p).
\]

(4)

We obtain the exact solution of the Hamiltonian from

\[
\Omega(E, p) = S_{11}(E, p) \cdot S_{33}(E, p) - S_{31}(E, p) \cdot S_{13}(E, p) = 0
\]

(5)

The four roots of \( \Omega(E, p) \) are the solutions of Eq. (1), \( E_{k \sigma}(p) \), which correspond to the two deepest coupled levels of the stepped QW \( (k = 1, 2) \), and their respective spin down and spin up sublevels \( (\sigma = \uparrow, \downarrow) \). We can identify spin orientation by means of the roots of \( S_{11}(E, p) \) and \( S_{33}(E, p) \). Roots of \( S_{11}(E, p) \) correspond to the two coupled sublevels with
spin up and $S_{33}(E,p)$ roots indicate spin down sublevels. The relative position of the roots helps us to know if we will get spin crossing or anticrossing.

For a wide range of $p$ values we obtain dispersion relations. We refer to them as quasi-paraboloids because pure paraboloid shape is broken at anticrossing points [4].

After obtaining coefficients $a_{\mu\sigma}$, $b_{\mu\sigma}$ (Eq. 2) we construct wave functions for each energy sublevel ($k\sigma$) and momentum $p$. If we denote by $\Psi^{\mu\kappa\sigma}(p,z)$ the wave function $\Psi^{\mu\sigma}(p,z)$ for a particular level $k$, then

$$
\Psi^{k\sigma}(p,z) = \sum_{\mu} \Psi^{\mu\kappa\sigma}(p,z) = \\
= \Theta(L1 - z)\Psi^{b\kappa\sigma}(p,z) + \Theta(z - L1)\Theta(L2 - z)\Psi^{w1\kappa\sigma}(p,z) + \\
+ \Theta(z - L2)\Theta(L3 - z)\Psi^{w2\kappa\sigma}(p,z) + \Theta(z - L3)\Psi^{b\kappa\sigma}(p,z),
$$

(6)

where $\Theta(z)$ is the Heaviside function. Finally, we normalize wave functions.

Next we will analyze the intersubband absorption coefficient. Because this coefficient is related to the transitions between occupied and empty sublevels, we have to include electron density effects, which determine occupied sublevels. Let’s remember that, till now, we have the one-electron solution. Actually, for doped systems Hamiltonian reads

$$
\varepsilon^{\mu}(p) + \frac{p^2}{2m^{\mu}} + U^{\mu}(z) + \hat{W}^{\mu}(p) + V^{H}(z) + V^{xc}(z),
$$

(7)

where $V^{H}(z)$, and $V^{xc}(z)$ are the Hartree, and the Fock potential terms, respectively. If we include the last potentials in Eq. (1), this equation has to be solved selfconsistently, together with the Poisson equation. Hartree potential is obtained from de Poisson equation in the usual manner,

$$
V^{H}(z) = \frac{4\pi e^2}{\epsilon} \int_{-\infty}^{z} dz^{'} (z - z^{'}) [N_{D}(z^{'}) - n_{e}(z^{'}).]
$$

(8)

Here $N_{D}(z)$ is the 3D doping profile of donors, $\epsilon$ is the dielectric permittivity that we have supposed as uniform across the heterostructure, and

$$
n_{e}(z) = \sum_{k\sigma} \int \frac{d\mathbf{p}}{(2\pi \hbar)^2} [\Psi^{k\sigma}(\mathbf{p},z)]^* \Psi^{k\sigma}(\mathbf{p},z) \Theta(\epsilon_{F} - E_{k\sigma}(\mathbf{p})).
$$

(9)

Thus, $\int n_{e}(z)dz = n_{2D}$ is the in-plane averaged 2D density of electrons and $k\sigma$ summatory extends to the occupied subbands. The Fermi energy $\epsilon_{F}$, is expressed through the total electron density $n_{2D}$, and depends on $H$ for a fixed concentration.
To simplify calculations we assume that, for sheet densities of the order of $10^{11} \text{ cm}^{-2}$ or lower, electron-electron interaction does not alter one-electron results substantially. Thus, we will neglect Fock term. For the Hartree potential, instead of using the momentum-dependent self-consistency (with the difficulties involved due to $\mathbf{p}$ dependence), we solve the above one-electron Hamiltonian but taking advantage of the Hartree effect that occurs in the electronic transitions. Hartree potential generates a noticeable shift in the frequency of intersubband electronic transitions. This change is because the photoexcitation electric field produces the superposition of wave functions of the subbands involved in transitions.

As a result, the charge density is no longer homogeneously distributed along the $z$ direction. The charge redistribution induces a space charge field that overlaps with the laser driving field and affects the interlevel distance. This process is known as depolarization [14–17]. We define the depolarization for the transition from $(k \sigma)$ to $(k' \sigma')$ as

$$
\delta_{k' \sigma' k \sigma} = \frac{8 \pi e^2}{\epsilon (E_{k' \sigma' k \sigma})} \int_{-\infty}^{\infty} dz \left[ \int_{-\infty}^{z} dz' \sum_{\mathbf{p}} \Psi_{k' \sigma'}^{\mathbf{p}}(0, z') \Psi_{k \sigma}^{\mathbf{p}}(0, z') \right]^2.
$$

(10)

where $E_{k' \sigma' k \sigma} = E_{k' \sigma'}(0) - E_{k \sigma}(0)$. Depolarization causes an interlevel energy shift which can be expressed as

$$
\tilde{E}_{k' \sigma' k \sigma} = E_{k' \sigma' k \sigma} (1 + \delta_{k' \sigma' k \sigma})^{1/2}
$$

(11)

### B. Intersubband optical absorption

To analyze the absorption coefficient we have adapted Ahn and Chuang expressions [18], obtained with matrix density formalism for parabolic dispersion relations. In our case we deal with non-parabolic dispersion relation and momentum-dependent integrals must be done numerically because the loss of symmetry in the $\mathbf{p}$-space. However, calculations are simplified because intersubband transitions between the fundamental and first excited subbands are induced only by light incident parallel to the growth plane [19]. To say, the polarization vector lies in the $z$ axis direction. In our case, the linear absorption coefficient for the optical transition between states $(k \sigma)$ and $(k' \sigma')$, as a function of the incident light frequency and for fixed transverse electric and in-plane magnetic fields, reads

$$
\alpha^{(1)}(\omega) = \omega \sqrt{\frac{\hbar}{\epsilon R V}} \sum_{k \sigma, k' \sigma'} \sum_{\mathbf{p}} |M_{k' \sigma' k \sigma}(\mathbf{p})|^2 \left[ f_{k \sigma}(\mathbf{p}) - f_{k' \sigma'}(\mathbf{p}) \right] \Gamma \left( \frac{\tilde{E}_{k' \sigma' k \sigma} - \hbar \omega}{\Gamma} \right)^2 + \Gamma^2.
$$

(12)
where

\[ M_{k'\sigma'k\sigma}(p) = |e| \langle k'\sigma' | z | k\sigma \rangle = |e| \int_{-\infty}^{\infty} zdz \left[ \Psi^{k'\sigma'}(p,z) \right]^* \Psi^{k\sigma}(p,z) \]  

are the dipole matrix elements, and

\[ f_{k\sigma}(p) = \frac{1}{1 + \exp \left[ \left( E_{k\sigma}(p) - \varepsilon_F \right) / k_B T \right]} \]  

is the well known Fermi-Dirac function for a Fermi energy \( \varepsilon_F \). The energy broadening of the absorption peaks is \( \Gamma = \hbar / \tau_r \) where \( \tau_r \) is the intersubband relaxation time. For simplicity, we take an unique value for all transitions. In Eq. (12) \( \mu \) is the permeability and \( \varepsilon_R \) is the real part of the permittivity (\( \varepsilon_R = \varepsilon_0 n_r^2 \)) of the wells (we take the same values for the two materials), \( n_r \) is the refractive index, \( c \) is the light speed in the vacuum, and \( V \) is the volume of the sample.

The third order nonlinear optical absorption is given by

\[
\alpha^{(3)}(\omega, I) = -\omega \sqrt{\mu / \varepsilon_R V} \left( \frac{2 I}{2 \varepsilon R c} \right) \times \\
\sum_{k\sigma,k'\sigma',p} |M_{k'\sigma'k\sigma}(p)|^4 \frac{\left[ f_{k\sigma}(p) - f_{k'\sigma'}(p) \right] \Gamma}{\left[ (\tilde{E}_{k'\sigma'k\sigma} - \hbar \omega)^2 + \Gamma^2 \right]^2} \times \\
\left\{ 4 - \frac{|M_{k'\sigma'k\sigma}(p) - M_{k\sigma k\sigma}(p)|^2}{|M_{k'\sigma'k\sigma}(p)|^2} \times \\
\frac{\left[ (\tilde{E}_{k'\sigma'k\sigma} - \hbar \omega)^2 - \Gamma^2 + 2\tilde{E}_{k'\sigma'k\sigma} (\tilde{E}_{k'\sigma'k\sigma} - \hbar \omega) \right]}{\left[ (\tilde{E}_{k'\sigma'k\sigma})^2 + \Gamma^2 \right]} \right\},
\]  

where \( I \) is the optical power per unit area. The total absorption coefficient is

\[ \alpha(\omega, I) = \alpha^{(1)}(\omega) + \alpha^{(3)}(\omega, I). \]  

Intersubband optical transitions between sublevels with the same spin (\( \sigma \rightarrow \sigma \)) are called spin conserving transitions, while those that occur between different spin sublevels (\( \sigma \rightarrow \sigma' \)) are often called spin flip transitions.

\[ III. \quad RESULTS \ AND \ DISCUSSION \]

The structure we use in the calculations consists of a stepped QW formed by a 400 Å wide QW of In\(_{0.9}\)Al\(_{0.1}\)Sb (\( w_1 \)) which includes a 50 Å wide QW of InSb (\( w_2 \)). The
structure is enclosed by $In_{0.8}Al_{0.2}Sb$ barriers. Data for this structure are $\Delta E_{c12} = 101.2$ meV, $\Delta E_{c2b} = 202.3$ meV (Fig. 1), $m_{w1} = 0.0246m_e$, $m_{w2} = 0.0142m_e$, and $m_b = 0.0352m_e$, where $m_e$ is the free electron rest mass [20, 21].

For this stepped QW resonance between ground and first excited conduction levels, in absence of magnetic field, is achieved around an electric field $F_\perp = 12.5$ meV. In addition to this transverse electric field we apply an in-plane magnetic field to get Zeeman splitting. We find the desired sublevels crossing for $H = 6$ T. For higher magnetic fields crossings will occurs at bigger $p$ values where first sublevel is empty. For lower magnetic fields there are not spin crossing. Thus, we also use $H = 4$ T to compare with the former case.

We consider the structure is selectively doped. To analyze concentration effects we use two density values, $n_{2D} = 8.25 \times 10^{10}$ cm$^{-2}$ and $n_{2D} = 3.6 \times 10^{11}$ cm$^{-2}$, corresponding to $\varepsilon_F = 103$ meV and $\varepsilon_F = 113$ meV, respectively.

A. Dispersion relations

First we look for eigenenergy values by means of Eq. (5). Energy sublevels correspond to the roots of $\Omega(E, p)$. As mentioned above, we identify spin up orientation from $S_{11}(E, p)$ and spin down from $S_{33}(E, p)$. Fig. 2(a) represents $\Omega(E, p)$, $S_{11}(E, p)$ and $S_{33}(E, p)$ versus $E$ for a momentum $p = 0$ and for $H = 6$ T, together with zero horizontal axis to display the location of the solutions. The two roots of lower energy correspond to spin down sublevels ($E_{1\downarrow}, E_{2\downarrow}$) followed by spin up sublevels ($E_{1\uparrow}, E_{2\uparrow}$). This indicates that spin splitting ($E_{1\uparrow} - E_{1\downarrow}$) is greater than the spacing between the electronic levels ($E_{2\downarrow} - E_{1\downarrow}$).

For a high enough momentum beyond the crossing, ($p_x/p_0 = 100$, e.g.), Fig. 2(b) shows the standard alternating spin orientations ($E_{1\downarrow}, E_{1\uparrow}, E_{2\downarrow}, E_{2\uparrow}$). This means a spin crossing occurs for some intermediate $p_x/p_0$ value. We take $p_0 = m_{w2}v_{w2}$ as a normalization factor to get dimensionless momentum.

Fig. 2(c) represents the same functions for $H = 4$ T and $p = 0$. Again we find ($E_{1\downarrow}, E_{1\uparrow}, E_{2\downarrow}, E_{2\uparrow}$). In this case we would find the same order for any $p$ value indicating there is no crossing of sublevels.

By repeating the process for a wide range of momenta we obtain the dispersion relations. Because of the difficulty presented by the quasi-paraboloids to see clearly spin crossings, we draw 2D sections of them, without loss of generality. Fig 3(a) shows $E_{k\sigma}$ versus $p_x/p_0$ for
$H = 6 \, \text{T}$ and $p_y = 0$. Arrows indicate position of anticrossings of the two spin orientations of each energy level. Due to the verticality of the curves in the region where they occur, deformation of the parabolas in the area can not be perceived. Since these anticrossings are not the aim of the present work we focus on the $\mathbf{p}$ region where crossings occurs. We present this zone in Fig. 3(b). Looking at $p_x = 0$, we can see the $(1 \uparrow)$ parabola is above the $(2 \downarrow)$ one. Since the curvature of the $(2\sigma)$ parabolas is greater than that of the $(1\sigma)$ parabolas and they shift in opposite directions along $p_x$ axis for different spin values, the crossing of spin sublevels $(1 \uparrow)$ and $(2 \downarrow)$ is obvious for a pair of momentum values. These spin crossings happen around $p_x/p_0 = -28$ and $p_x/p_0 = 54$. Beyond these momenta the normal spin order is recovered. For an analogous region, Fig. 3(c) shows $E_{k\sigma}$ versus $p_y/p_0$ for $p_x = 0$. Now, spin crossings are symmetrically placed at $p_y/p_0 = \pm 39$.

In order to compare with the case where no spin crossings exist, we represent in Fig. 4(a) and 4(b) relation dispersion for $H = 4 \, \text{T}$. As can be seen, in this case the $(1 \uparrow)$ parabola is under the $(2 \downarrow)$ one, following the usual behavior. Although these parabolas approximate each other and it would seem that they are crossing, the different curvature of parabolas leads to no crossing at all.

Once obtained dispersion relations we calculate and normalize wave functions $\Psi^{k\sigma}(\mathbf{p},z)$. As an example Fig. 5 shows the case for $H = 6 \, \text{T}$ and $\mathbf{p} = 0$. Due to the applied electric field $F_\perp = 12.5 \, \text{kV/cm}$, just after resonance, the first level is mainly located in the left side of the wide well, whereas the second level basically corresponds to the narrow well. In both cases sublevels $\sigma = \uparrow$ are more confined in their corresponding wells, while sublevels $\sigma = \downarrow$ are more distributed between the two wells. This behavior will affect the overlap of wave functions and thus, the depolarization shift of transitions frequency.

### B. Spin intersubband absorption

Next, we calculate dipole matrix elements $M_{k'\sigma'k\sigma}(\mathbf{p})$ and, finally, the total absorption coefficient taking into account both linear $\alpha^{(1)}(\omega)$ and non-linear $\alpha^{(3)}(\omega, I)$ contributions. We take $\Gamma = 1 \, \text{meV}$, $T = 4.2 \, \text{K}$, $n_r = 4$, and $I = 1 \, \text{MW/cm}^2$.

First, we consider $n_{2D} = 8.25 \times 10^{10} \, \text{cm}^{-2}$ corresponding to $\varepsilon_F = 103 \, \text{meV}$. In this case only the deepest spin sublevel is occupied, as can be seen in Figs. 3(b-c) and 4(a-b), for $H = 6 \, \text{T}$ and $H = 4 \, \text{T}$, respectively. In these figures, Fermi level is represented by the
dotted line. Paraboloids corresponding to the three higher sublevels have energies greater than Fermi energy and are empty. However, the deepest sublevel is below Fermi energy in a certain momentum range. Electrons occupy this region of the bottom of the paraboloid.

Fig. 6 shows total absorption coefficient for $\varepsilon_F = 103$ meV and when only the $(1 \downarrow)$ sublevel is occupied. Fig. 6(a) presents the $H = 6$ T case, where there is a spin crossing of sublevels. Absorption spectrum shows three peaks corresponding to transitions from this $(1 \downarrow)$ sublevel to the other three empty sublevels $(2 \downarrow)$, $(1 \uparrow)$ and $(2 \uparrow)$, respectively, in increasing order of energy. The first is a spin-conserving transition while the other two are spin flip transitions. Fig. 6(b) presents the other case, $H = 4$ T, when there is not such a crossing. Now, absorption spectrum displays two dominant peaks, corresponding to transitions from $(1 \downarrow)$ to $(1 \uparrow)$ and $(2 \uparrow)$. The third peak, for the transition $(1 \downarrow)$ to $(2 \downarrow)$ is too small compared with the others and can not be noticed in the total spectrum.

For $n_{2D} = 3.6 \times 10^{11}$ cm$^{-2}$, corresponding to $\varepsilon_F = 113$ meV, and due to levels proximity, we have three occupied sublevels. This situation is also represented in dispersion relation figures [Figs. 3(b-c) and 4(a-b)], where dash-dotted lines correspond to this Fermi energy value. Unlike the previous case, now only paraboloid corresponding to the highest sublevel has energy greater than Fermi energy and is the only one fully empty. Nevertheless, the other three sublevels cut the Fermi energy for some momentum values leading to the occupation of the bottom of paraboloids with $E_{k\sigma}(p) < \varepsilon_F$. For higher $|p|$ values there is an empty lateral region for $E_{k\sigma}(p) > \varepsilon_F$. In 2D figures it can be seen as little regions on left and right of the dispersion relations but, actually, it is a thin ring in 3D paraboloids.

Fig. 7 presents absorption coefficient for $\varepsilon_F = 113$ meV. Now, only sublevel $(2 \uparrow)$ is empty and transitions go from the others sublevels to it. We have also considered the little regions where sublevels $(1 \uparrow)$ and $(2 \downarrow)$ lay over Fermi energy level, while sublevel $(1 \downarrow)$ is under it. Thus, there are two possible transitions between these sublevels in this $p$-region, from the deepest one $(1 \downarrow)$ to the sublevels $(1 \uparrow)$ and $(2 \downarrow)$. Nevertheless, results show that the peaks of these transitions are negligible compared with the others and are not visible in the total spectrum. Fig. 7(a) presents the "spin crossing case", for $H = 6$ T. As in the former situation, we find three peaks corresponding to transitions from sublevels $(1 \uparrow)$, $(2 \downarrow)$ and $(1 \downarrow)$ to sublevel $(2 \uparrow)$, respectively, in the same increasing order of energy. Fig. 7(b) shows the $H = 4$ T case, where there is not spin crossing. In a similar way as found before, we can appreciate only two peaks, because the corresponding to spin-flip transition
from \((2 \downarrow)\) sublevel to \((2 \uparrow)\) one is smaller and, due to depolarization shift, almost coincides with the transition from \((1 \uparrow)\) sublevel, resulting in a single peak in the total spectrum. The other peak for the transition from \((1 \downarrow)\) to \((2 \uparrow)\) seems to be similar for the two cases, since spin crossing sublevels are not involved.

This behavior of the peaks, caused by the polarization shift, can also be seen for \(\epsilon_F = 103\) meV in Fig. 6(b). The small peak corresponding to spin-conserving transition \((1 \downarrow)\) to \((2 \downarrow)\), besides being hardly visible in the total spectrum, almost coincides with the spin-flip transition \((1 \downarrow)\) to \((1 \uparrow)\).

Considering the four cases under study we can see a general behavior both for transitions from an unique occupied spin sublevel \([((1 \downarrow) \rightarrow (1 \uparrow), (2 \downarrow), (2 \uparrow))]\), and for transitions up to an unique empty sublevel \([((1 \downarrow), (1 \uparrow), (2 \downarrow) \rightarrow (2 \uparrow))]\), as Figs. 6 and 7 show. The transition between the lower and higher sublevels \([((1 \downarrow) \rightarrow (2 \uparrow))]\) gives rise to the dominant absorption peak in every case, specially for higher electronic density. Because of the involved sublevels are not susceptible of crossing, their behavior is similar for both magnetic fields used.

Sublevels \((1 \uparrow)\) and \((2 \downarrow)\) are close together in energy. This would lead to the nearness of the transitions involved: \([((1 \downarrow) \rightarrow (1 \uparrow), (2 \downarrow))]\) and \([((1 \uparrow), (2 \downarrow) \rightarrow (2 \uparrow))]\) (for \(\epsilon_F = 103\) meV and \(\epsilon_F = 113\) meV, respectively), and only one peak would be observable. However, when considering the depolarization shift of transitions, absorption peaks separate each other and become distinguishable in the spin crossing case. Depolarization shift depends on wave functions overlapping. It can be proved that wave functions overlap corresponding to spin sublevels of the same electronic level is very much greater than that of sublevels of different electronic levels. This fact is reflected in the different energy shift of the corresponding absorption peaks, which is greater for transitions \([((1 \downarrow) \rightarrow (1 \uparrow))\) and \([((2 \downarrow) \rightarrow (2 \uparrow))]\) than for transitions \([((1 \downarrow) \rightarrow (2 \downarrow))]\) and \([((1 \uparrow) \rightarrow (2 \uparrow))]\).

When spin crossing exists and for \(\epsilon_F = 103\) meV [Fig. 6(a)], absorption peaks follow the order in energy \([((1 \downarrow) \rightarrow (2 \downarrow)), (1 \downarrow) \rightarrow (1 \uparrow))]\). By considering shift caused by depolarization, displacement of second transition \([((1 \downarrow) \rightarrow (1 \uparrow))]\) is much greater than that of the first one and both peaks separate each other and become clearly visible in the total spectrum. A similar situation occurs for \(\epsilon_F = 113\) meV [Fig. 7(a)], where the order of transitions is \([((1 \uparrow) \rightarrow (2 \uparrow)), (2 \downarrow) \rightarrow (2 \uparrow))]\). Again, peak corresponding to second transition shifts more than that of the other and both are discernible.

When there is not spin crossing the position of the transitions is inverted [Figs. 6(b) and
In this case, the larger displacement of the first peak makes it almost coincident with the second one, showing an unique peak for both transitions. Results are in agreement with available experimental data for the case where there is not spin sublevel crossing and other theoretical works for stepped quantum wells.

In short, the existence of spin sublevel crossing changes the energy order of the electron transitions which, together with the depolarization shift, provides an additional peak in the structure of the absorption spectrum.

IV. CONCLUSIONS

In this work we present a modified version of the Transfer Matrix Approach which includes transverse electric field, in-plane magnetic field and abrupt interfaces. Together with first order boundary conditions we construct a momentum dependent pseudo Wronskyan matrix to obtain non-parabolic dispersion relations. We consider Zeeman splitting of electronic levels in InSb-based stepped quantum wells. For certain values of the magnetic field we find spin sublevel crossing or quasi-paraboloids intersection. We calculate linear and non-linear intersubband optical absorption coefficients including electron density effects through the displacements of transitions caused by depolarization. We find that the spin crossing modifies absorption spectrum showing an additional peak when compared with the standard non crossing situation.

The present method has proved to be effective in the study of spin properties such as spin anticrossing and spin crossing. A similar theoretical analysis may be developed for other structures under magnetic field. We hope that present results will stimulate experimental efforts towards the study of spin crossing peculiarities in nanostructures.

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FIGURE CAPTIONS

Figure 1. Scheme of the stepped quantum well with the two deepest resonant levels and their corresponding spin splitting.

Figure 2. $\Omega (E, p)$ (red solid line), $S_{11} (E, p)$ (dotted green line) and $S_{33} (E, p)$ (dashed blue line) versus $E$. (a) $H = 6$ T, $p = 0$. (b) $H = 6$ T, $p_x/p_0 = 100$, $p_y = 0$. (c) $H = 4$ T, $p = 0$.

Figure 3. Dispersion relations for $H = 6$ T. (a) Energy vs dimensionless $p_x$ for $p_y = 0$. Arrows indicate anticrossing regions. (b) Magnification of the central area of the previous dispersion relation showing the spin crossing. (c) Energy vs dimensionless $p_y$ for $p_x = 0$. Dotted line: $\varepsilon_F = 103$ meV, and dash-dotted line: $\varepsilon_F = 113$ meV.

Figure 4. Dispersion relations for $H = 4$ T. (a) Energy vs dimensionless $p_x$ for $p_y = 0$. (b) Energy vs dimensionless $p_y$ for $p_x = 0$. Dotted line: $\varepsilon_F = 103$ meV, and dash-dotted line: $\varepsilon_F = 113$ meV.

Figure 5. Wave functions for $H = 6$ T and $p = 0$.

Figure 6. Intersubband optical absorption for $\varepsilon_F = 103$ meV. (a) $H = 6$ T. (b) $H = 4$ T.

Figure 7. Intersubband optical absorption for $\varepsilon_F = 113$ meV. (a) $H = 6$ T. (b) $H = 4$ T.
Figure 1

FIG. 1: Scheme of the stepped quantum well with the two deepest resonant levels and their corresponding spin splitting.
Figure 2(a)
Figure 2(b)
FIG. 2: $\Omega (E, p)$ (red solid line), $S_{11} (E, p)$ (dotted green line) and $S_{33} (E, p)$ (dashed blue line) versus $E$. (a) $H = 6 \, T$, $p = 0$. (b) $H = 6 \, T$, $p_x/p_0 = 100$, $p_y = 0$. (c) $H = 4 \, T$, $p = 0$. 

Figure 2(c)
Figure 3(a)

\[ E_{k_\sigma} \text{ (meV)} \]

\[ p_x/p_0 \]
Figure 3(b)
FIG. 3: Dispersion relations for $H = 6$ T. (a) Energy vs dimensionless $p_x$ for $p_y = 0$. Arrows indicate anticrossing regions. (b) Magnification of the central area of the previous dispersion relation showing the spin crossing. (c) Energy vs dimensionless $p_y$ for $p_x = 0$. Dotted line: $\varepsilon_F = 103$ meV, and dash-dotted line: $\varepsilon_F = 113$ meV.
Figure 4(a)
FIG. 4: Dispersion relations for $H = 4$ T. (a) Energy vs dimensionless $p_x$ for $p_y = 0$. (b) Energy vs dimensionless $p_y$ for $p_x = 0$. Dotted line: $\epsilon_F = 103$ meV, and dash-dotted line: $\epsilon_F = 113$ meV.
FIG. 5: Wave functions for $H = 6$ T and $p = 0$. 

Figure 5
Figure 6(a)
FIG. 6: Intersubband optical absorption for $\varepsilon_F = 103$ meV. (a) $H = 6$ T. (b) $H = 4$ T.
Figure 7(a)
FIG. 7: Intersubband optical absorption for $\varepsilon_F = 113$ meV. (a) $H = 6$ T. (b) $H = 4$ T.