Influence of spin-orbit interaction on quantum cascade transitions

Vadim M. Apalkov
Department of Physics and Astronomy, Georgia State University, Atlanta, Georgia 30303, USA and Department of Physics and Astronomy, University of Manitoba, Winnipeg, Canada R3T 2N2

Anjana Bagga and Tapash Chakraborty*
Department of Physics and Astronomy, University of Manitoba, Winnipeg, Canada R3T 2N2
(Dated: November 11, 2018)

We have investigated the effect of spin-orbit (SO) coupling on the emission spectra of a quantum cascade laser. In an externally applied magnetic field parallel to the electron plane, the SO coupling would result in a double-peak structure of the optical spectra. This structure can be observed within some interval of magnetic fields and only for diagonal optical transitions when the SO coupling is different in different quantum wells.

PACS numbers: 42.55.Px, 71.70.Ej, 73.21.Fg

The quantum cascade laser (QCL) is a coherent source of infrared radiation and also an ingenious demonstration of quantum confinement and tunneling in quantum well structures [1, 2]. These are specially designed superlattices of quantum wells. Optical transitions between the subband levels of dimensional quantization in the growth direction of QCL occur within the active region. In these subbands, motion of electrons in the growth direction is frozen and electron motion is two-dimensional. The electron states within each subband are characterized by a two-dimensional momentum, \( \mathbf{k} \), and optical transitions between subbands are allowed only between the states with the same momentum \( \mathbf{k} \) and the same spin projection. It is now well established that a strongly asymmetric confinement potential results in a spin-orbit (SO) coupling [3]. Many novel effects that are entirely due to the SO interaction have been proposed and some are observed experimentally [1, 2, 3]. In this paper we analyze the possible effects of SO coupling on the optical emission of the QCL.

Since the SO interaction couples the orbital motion and spin one would expect that SO coupling should produce two types of optical lines, corresponding to transitions between the same spin orientation of the two subbands and between the different spin orientations. However, for a weak enough disorder only one type of transition is allowed. This is because, for the SO interaction \( \alpha (\mathbf{k} \times \mathbf{\sigma}) \mathbf{n} \), where \( \alpha \) is the SO coupling constant, \( \mathbf{\sigma} \) is the spin operator, and \( \mathbf{n} \) is the unit vector normal to the two-dimensional plane [3], the spin direction is correlated with the direction of momentum and the spin states will be characterized by definite values of the chirality, i.e. the spin projection on the direction perpendicular to \( \mathbf{k} \). For a weak disorder the optical transitions are allowed only between the states with the same \( \mathbf{k} \). Then the requirement of spin conservation during optical transitions allows only transitions between the states with the same chirality, i.e. only a single optical line should be observed.

To observe the two optical lines we need to modify the energy spectra of electrons in different subbands. One way of doing this is by applying a parallel magnetic field. Since we are studying the qualitative effects of SO coupling on the optical spectra of the QCL we consider only two subbands in the active region of the QCL. Electrons in these subbands will have different positions in the growth direction of QCL. In other words, denoting the growth direction as \( z \)-axis, we assume that \( z_u = \langle z \rangle \) (the average value of \( z \) for the upper subband) is different from \( z_l = \langle z \rangle \) (that of the lower subband). The values of \( z_u \) and \( z_l \) depends on the structure of the QCL and on the applied voltage. We will consider these quantities as parameters of the problem. We also assume that electrons occupy only the higher subband, and they are in quasi-equilibrium with temperature \( T \) and electron density \( n_s \). The wavefunctions of electrons in the upper and lower subbands will then have the form \( \Psi_u(x,y,z) = \psi_u(x,y) \chi_u(z) \) and \( \Psi_l(x,y,z) = \psi_l(x,y) \chi_l(z) \). Optical transitions between the upper and lower subbands will then determine the emission spectra of the QCL. The intensity \( I \) of these transitions is proportional to \( | \langle \chi_u | z | \chi_l \rangle \langle \psi_u | \psi_l \rangle |^2 \). Since the SO coupling should manifest itself in the \( x,y \)-planar dynamics we shall study below only the \( x,y \) part of this expression.

To get a large SO coupling the quantum wells (QWs) in the active region should be asymmetric. For such a structure the observed values of the SO coupling constant lie in the range of 5 - 45 meV nm [7]. With an applied parallel magnetic field the Hamiltonian describing the electron dynamics in the \( x,y \) plane for upper and lower subbands is [8]

\[
\mathcal{H}_s = \frac{1}{2m^*} \left( \vec{p} - \frac{e}{c} \vec{A} \right)^2 + \frac{\alpha_s}{\hbar} \left( \left[ \vec{p} - \frac{e}{c} \vec{A} \right] \times \hat{n} \right) \cdot \hat{n} - \frac{1}{2} g \mu_B B \sigma_y, 
\]

where the index \( s = u,l \) stands for upper and lower sub-
FIG. 1: Emission spectra for different values of the parallel magnetic field and for \( \alpha_s = -\alpha_l = 45 \) meV nm (left panel) and the corresponding energy spectra of upper and lower subbands as a function of \( k_x \) for \( k_y = 0 \) (right panel). States with a positive value of \( y \) projection of spin (solid lines), and with a negative value (dotted line) are also shown. The arrows illustrate two types of transitions which results in two-peak structure of emission spectra. The letters “u” and “l” next to the lines stand for upper and lower subbands, respectively.

bands respectively, \( \vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \) is the vector of Pauli spin matrices, \( \alpha_s \) is the SO coupling constant for an electron in the \( s \)-th subband, and \( m^* \) is the electron effective mass. In Eq. (1) we assumed that the SO coupling is different in different subbands, an important assumption since only in this case we could get the well-resolved double-peak structure of the optical spectra. Different values of \( \alpha \) in different subbands correspond to diagonal optical transition, i.e. the electrons in upper and lower subbands are localized in different quantum wells. Magnetic field in Eq. (1) is applied in the \(-\hat{y}\) direction. As a next step we introduce the gauge \( \vec{A} = (-Bz, 0, 0) \) and replace \( z \) by its average value \( z_s \) for the \( s \)-th subband. Then the eigenfunctions of the Hamiltonian [Eq. (1)] are classified according to the chirality, \( \kappa = \pm 1 \), and form two branches of the spectrum

\[
E_{s, \kappa}(\vec{k}) = \frac{\hbar^2}{2m^*} \left[ k_y^2 + \left( k_x + \frac{\omega}{\ell_B} \right)^2 \right] + \kappa \alpha_s \sqrt{\left( k_x + \frac{\omega}{\ell_B} \right)^2 + k_y^2}, \tag{2}
\]

where \( \ell_B = (\hbar/eB)^{1/2} \) is the magnetic length. The corresponding eigenfunctions are

\[
\psi_{s, \kappa}(\vec{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i\kappa \exp\left(i\phi_{s, \kappa} \right) \end{pmatrix} e^{ik_x x + ik_y y}, \tag{3}
\]

where the angle \( \phi_{s, \kappa} \) is related to \( \vec{k} \) as

\[
\tan \phi_{s, \kappa} = \frac{k_y + z_s/\ell_B^2 + 2\gamma \mu_B B/\alpha_s}{k_x + z_s/\ell_B^2 + 2\gamma \mu_B B/\alpha_s}. \tag{4}
\]

Taking into account the spin conservation during the optical transitions we can write the emission spectra as

\[
I(\omega) = I_0 \int \frac{d\vec{k}}{(2\pi)^2} \sum_{\kappa_1, \kappa_2} \left| f \left[ E_{u, \kappa_1}(\vec{k}) \right] \right|^2 \times \left| 1 + \kappa_1 \kappa_2 \exp\left(i\phi_{u, \kappa_1} - \phi_{u, \kappa_2}\right) \right|^2 \times \delta \left( E_{u, \kappa_1}(\vec{k}) - E_{l, \kappa_2}(\vec{k}) - \hbar\omega \right), \tag{5}
\]

where \( f(\epsilon) = 1/\left(\exp(\epsilon - \mu_F)/k_B T + 1\right) \) is the Fermi distribution function for electrons in the upper subband with the chemical potential \( \mu_F \), which corresponds to electron density \( n_s \) and temperature \( T \). It is easy to see that for zero parallel magnetic field, \( \phi_{u, \kappa} = \phi_{l, \kappa} \) and the spin part in Eq. (5) is non-zero only for \( \kappa_1 = \kappa_2 \). In this case optical transitions are allowed only between the states with the same chirality \( \kappa \). This is also the case when the magnetic field is large enough so that the Zeeman term in the Hamiltonian becomes larger than the SO term. Transitions between different subbands are allowed for intermediate values of the magnetic field, although the main transitions still come from the states with the same chirality. For a high density of electrons on the upper subband these transitions should give only a single line even in the presence of a parallel magnetic field. This situation can be changed if the population of the upper subband is low enough so that the electrons occupy states with the lowest energy. In the momentum space these states correspond to a circle with radius \( \alpha_s m^*/\hbar^2 \). It is easy to analyze this case by fixing the value at \( k_y = 0 \) and studying the spectra as a function of \( k_x \). Then the energy \( E_{u, \kappa}(k_x) \) has two minima and transitions from these minima can give rise to two peaks. The natural requirement to resolve these peaks is that the width of the peaks should be smaller than the separation between them. The maximum separation between the peaks will occur when the SO coupling constants \( \alpha_s \) have different signs in the upper and lower subbands.

To analyze the possibility to observe SO-induced two-peak structure of the emission spectra of a QCL we have calculated the optical spectra from Eq. (5) for the smallest density of electrons on the upper subband \( n_s = 10^{10} \) cm\(^{-2} \). To have the largest SO coupling constant, \( \alpha \approx 45 \) meV nm, we assume that the QCL is based on the narrow gap semiconductor, viz. InAs (\( m^*/m = 0.042 \) and \( g = -14 \)). We have also fixed the difference \( |z_u - z_l| \) at 3 nm and study the optical spectra as a function of the magnetic field. For illustration purpose we introduce the finite energy difference between the energy levels (upper and lower subbands) of the size quantization in the \( z \) direction to be 20 meV. This means that without the SO coupling and without a parallel magnetic
field the emission spectra consists of a single line centered at 20 meV.

In Fig. 1 the emission spectra are shown for $\alpha_u = -\alpha_l = 45$ meV.nm and for different values of the parallel magnetic field. In the right panel the energy spectra of upper and lower subbands are shown as a function of $k_x$ for $k_y = 0$. For $k_y = 0$ the electron subbands can be classified by the definite value of $y$-projection of the spin, $\sigma_y$. The solid lines correspond to the positive value of spin, while the dotted lines correspond to the negative values. Due to the small electron density in the upper subbands only the lowest states are occupied. Because of the SO coupling electrons in these states will have different directions of spin in different regions of $k_x$. For example, for $k_x$ to the right from the point of intersection of two branches the spin is positive, while for $k_x$ to the left the spin is negative. Transitions from these two types of electron states can produce the two-peak emission spectra. These transitions are shown by arrows in Fig. 1. At small values of the magnetic field these peaks almost coincide and a small shoulder emerges due to allowed optical transition to the ground state. Eventually, with increasing $B$ two peaks can be resolved and at $B \approx 2.2T$ they have the same intensity. At even larger $B$ the intensity of one of the peak will be suppressed and the optical spectrum again acquires a single-peak structure.

With increasing magnetic field the Zeeman energy becomes stronger and only the states with negative spin is occupied. As a result, there is only a single peak. This peak will be initially blue shifted by an amount $\sim 5$ meV from the zero magnetic field peak and then for a weak enough disorder it will be red shifted as in the absence of any SO coupling \[3\].

The condition $\alpha_u = -\alpha_l$ results in the strongest separation between two peaks. For smaller difference between $\alpha_u$ and $\alpha_l$ the two-peak structure becomes less pronounced and finally it will disappear at $\alpha_u = \alpha_l$. The evolution of the two-peak emission spectra with decreasing difference between $\alpha_u$ and $\alpha_l$ is shown in Fig. 2, together with the energy spectra of upper and lower subbands. For $\alpha_u = 0$ and $\alpha_l = 45$ meV.nm the strongest effect that we can get at some value of the magnetic field is the shoulder in the emission spectra \[Fig. 2(b)\]. For $\alpha_u = \alpha_l$, and for all values of the magnetic field there is only a single peak \[Fig. 2(c)\]. While in this case there are also two types of transitions, the width of the corresponding peaks are larger then the separation between them. The inset in Fig. 2 illustrates schematically the structure of two wells which gives the corresponding relation between the SO coupling, where the upper and lower states are localized in different wells.

In Fig. 3 the evolution of a two-peak structure of the emission spectra with change of SO coupling is shown for $\alpha_u = -\alpha_l$. The magnetic field at which the two-peak structure becomes most pronounced is different for different values of $\alpha_u$. With decreasing $\alpha_u$ the separation between the peaks decreses and finally at small values of $\alpha_u$ two peaks could not be resolved.

In conclusion, we have shown that the SO coupling in QCL could result in a two-peak structure of the emission spectra. To observe such a structure, the quantum wells constituting the active region of QCL should be asymmetric and optical transitions should be diagonal. The next important condition is that SO couplings in different quantum wells should be very different. In this case a two-peak emission line can be developed within some interval of a parallel magnetic field. Since in the para-

---

*FIG. 2: Emission spectra for different structure of active region of QCL (left panel), which result in different values of SO coupling in upper and lower subbands: (a) $\alpha_l = -\alpha_u = 45$ meV.nm, (b) $\alpha_u = 0$ and $\alpha_l = 45$ meV.nm, (c) $\alpha_l = \alpha_u = 45$ meV.nm. The schematic illustration of corresponding active regions are shown as an inset. The corresponding energy spectra of upper and lower subbands as a function of regions are shown as an inset. The corresponding energy spectra of upper and lower subbands only the lowest states are occupied. Because of spin, while the dotted lines correspond to the negative value of $y$-projection of spin (solid lines) and those with negative value (dotted line) are also shown.*

*FIG. 3: Emission spectra for different values of $\alpha_u$ and the magnetic field under the condition $\alpha_l = -\alpha_u$: $\alpha_u = 20$ meV.nm and $B = 0.8$ tesla (solid line), $\alpha_u = 45$ meV.nm and $B = 2.2$ tesla (dotted line), and $\alpha_u = 60$ meV.nm and $B = 3.24$ tesla (dashed line).*
magnetic field the occupation of the upper subband determine the width of the optical lines, to resolve the two-peak structure the electron density and the temperature should be small enough, so that the width of the lines is less than the separation between them.

The work of T.C. has been supported by the Canada Research Chair Program and the Canadian Foundation for Innovation Grant.

[1] C. Gmachl, F. Capasso, D.L. Sivco, and A.Y. Cho, Rep. Prog. Phys. 64, 1533 (2001).
[2] T. Chakraborty and V.M. Apalkov, Adv. Phys. 52, 455 (2003).
[3] Yu. A. Bychkov and E. I. Rashba, Pis’ma Zh. Eksp. Teor. Fiz. 39, 64 (1984) [JETP Lett. 39, 78 (1984)].
[4] D.D. Awschalom, D. Loss, and N. Samarth (Eds.), Semiconductor Spintronics and Quantum Computation (Springer, 2002); D. Grundler, Phys. World 15, 39 (2002); S.A. Wolf, D.D. Awschalom, R.A. Buhrman, J.M. Daughton, S. von Molnar, M.L. Roukes, A.Y. Chtchelkanova, and D.M. Treger, Science 294, 1488 (2001); G.A. Prinz, Phys. Today 48, 58 (1995).
[5] Proceedings of the First International Conference on the Physics and Applications of Spin Related Phenomena in Semiconductors, edited by H. Ohno [Physica E 10 (2001)].
[6] T. Chakraborty and P. Pietiläinen, Phys. Rev. B 71, 113305 (2005); M. Califano, T. Chakraborty and P. Pietiläinen, Phys. Rev. Lett. 94, 246801 (2005); Appl. Phys. Lett. (to be published).
[7] D. Grundler, Phys. Rev. Lett. 84, 6074 (2000); C.-M. Hu, J. Nitta, T. Akazaki, H. Takayanagi, J. Osaka, P. Pfeiffer, and W. Zawadzki, Phys. Rev. B 60, 7736 (1999); T. Matsuyama, C.M. Hu, D. Grundler, G. Meier, and U. Merkt, Phys. Rev. B 65, 155322 (2002); J. Nitta, T. Akazaki, H. Takayanagi, and T. Enoki, Phys. Rev. Lett. 78, 1335 (1997); G. A. Khodaparast, R.E. Doezema, S.J. Chung, K.J. Goldammer, and M.B. Santos, Phys. Rev. B 70, 155322 (2004).
[8] V.M. Apalkov and T. Chakraborty, Appl. Phys. Lett. 78, 697 (2001).