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Spin-orbit interaction in a quantum cascade transition

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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 quantum well plane, the SO coupling results in a double-peak structure of the optical spectra. This structure could be observed within some interval of the magnetic field and only for diagonal optical transitions, when the SO coupling is different in different quantum wells.

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The quantum cascade transitions[1] occur in the quantum cascade laser (QCL), which is a coherent source of infrared radiation and also an ingenious demonstration of quantum confinement and tunneling in quantum well structures.[2] These are specially designed superlattices of quantum wells. Optical transitions between the subband levels of dimensional quantization in the growth direction of the QCL occur within the active region. In these subbands, the motion of electrons in the growth direction is frozen and electron motion is, to a good approximation, two dimensional. The electron states within each subband are characterized by a two-dimensioanl momentum, $\mathbf{k}$, and optical transitions between subbands are allowed only between 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.[4–7] In this paper we have investigated the possible effects of the SO coupling on the optical emission in a QCL.

Since the SO interaction couples the orbital motion and spin, one would expect that the 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 $\alpha(\mathbf{k}\times\boldsymbol{\sigma})\mathbf{n}$, where α is the SO coupling constant, $\boldsymbol{\sigma}$ 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.[8] The effect of a magnetic field on the optical and transport properties of quantum well structures has been studied extensively for different systems.[9,10] The main effect of this field is the momentum shift of the electron dispersion. This fact can strongly influence the processes, such as tunneling and optical transitions, where the conservation of two-dimensional momentum is involved. In optics this results, for example, in the shift of resonance lines and its broadening.[8,11]

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 the QCL. In other words, denoting the growth direction as the 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 depend 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 quasiequilibrium with temperature T and electron density n_s. The wave functions 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.[6,7] With an applied parallel magnetic field, the Hamiltonian describing the electron dynamics in the $x-y$ plane for upper and lower subbands is[3]

$$\mathcal{H}_s=\frac{1}{2m^*}(\mathbf{p}+e\mathbf{A})^2+\frac{\alpha_s}{\hbar}([\mathbf{p}+e\mathbf{A}]\times\boldsymbol{\sigma})\mathbf{n}+\frac{1}{2}g\mu_B B\sigma_y, \tag{1}$$

where the index $s=u,l$ stands for upper and lower subbands, respectively, $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ is the vector of Pauli spin matri-

ces, α_s is the SO coupling constant for an electron in the sth subband, m^* is the electron effective mass, and the charge of the electron is $-e$. In Eq. (1), the SO coupling is assumed to be different in different subbands, as only in this case we could get the well-resolved double-peak structure of the optical spectra. Different values of α in different subbands correspond to diagonal optical transition, i.e., the electrons in upper and lower subbands are localized in different quantum wells. The magnetic field in Eq. (1) is applied in the $\hat{y}$ direction. As a next step we introduce the gauge $\mathbf{A}=(Bz,0,0)$ and replace z by its average value z_s for the sth subband. Then the eigenfunctions of the Hamiltonian (1) are classified according to the chirality, $\kappa=\pm 1$, and form two branches of the spectrum

$$E_{s,\kappa}(\mathbf{k}) = \frac{\hbar^2}{2m^*}\left[k_y^2 + \left(k_x + \frac{z_s}{l_B^2}\right)^2\right] + \kappa\alpha_s\sqrt{\left(k_x + \frac{z_s}{l_B^2} + \frac{1}{2}\frac{g\mu_B B}{\alpha_s}\right)^2 + k_y^2}, \quad (2)$$

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

$$\psi_{s,\kappa}(\mathbf{k}) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i\kappa\exp(i\phi_{s,\mathbf{k}}) \end{pmatrix} e^{ik_x x + ik_y y}, \quad (3)$$

where the angle $\phi_{s,k}$ is related to $\mathbf{k}$ as

$$\tan\phi_{s,\mathbf{k}} = \frac{k_y}{k_x + z_s/l_B^2 + \frac{1}{2}g\mu_B B/\alpha_s}. \quad (4)$$

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

$$\begin{aligned} I(\omega) &= I_0\int\frac{d\mathbf{k}}{(2\pi)^2}\sum_{\kappa_1\kappa_2} f[E_{u,\kappa_1}(\mathbf{k})] \\ &\quad\times|\psi^\dagger_{u,\kappa_1}(\mathbf{k})\psi_{d,\kappa_2}(\mathbf{k})|^2\delta[E_{u,\kappa_1}(\mathbf{k}) - E_{l,\kappa_2}(\mathbf{k}) - \hbar\omega] \\ &= I_0\int\frac{d\mathbf{k}}{(2\pi)^2}\sum_{\kappa_1\kappa_2} f[E_{u,\kappa_1}(\mathbf{k})]|1+\kappa_1\kappa_2 e^{i(\phi_{u,\mathbf{k}}-\phi_{l,\mathbf{k}})}|^2 \\ &\quad\times\delta(E_{u,\kappa_1}(\mathbf{k}) - E_{l,\kappa_2}(\mathbf{k}) - \hbar\omega), \end{aligned} \quad (5)$$

where $f(\epsilon)=1/[\exp(\epsilon-\mu_F)/k_BT+1]$ is the Fermi distribution function for electrons in the upper subband with the chemical potential μ_F, which corresponds to electron density n_s and temperature T. In our calculations, the temperature was set to 1 K. It is easy to see that for a vanishing parallel magnetic field, $\phi_{u,\mathbf{k}}=\phi_{l,\mathbf{k}}$, and the spin part in Eq. (5) is nonzero only for $\kappa_1=\kappa_2$. In this case optical transitions are allowed only between the states with the same chirality κ. 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 is changed if the population of the upper subband is made 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 lowest energy branch $E_{u,\kappa}(k_x)$ [e.g., for $\alpha_u>0$ it is $E_{u,-1}(k_x)$] 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 α_s have different signs in the upper and lower subbands.

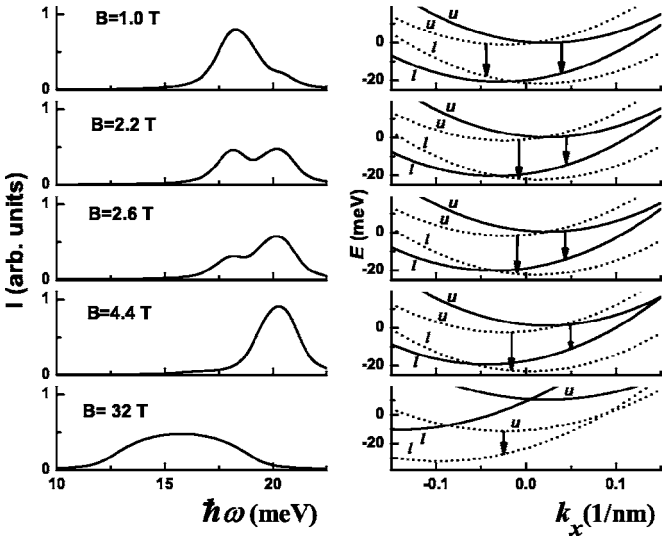

FIG. 1. Emission spectra for different values of the parallel magnetic field and for $\alpha_u=-\alpha_l=45$ meV nm (left panel) and the corresponding energy spectra of upper and lower subbands as a function of k_x for $k_y=0$ (right panel). States with a positive value of the y projection of spin (solid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

To analyze the possibility of observing a SO-induced two-peak structure of the emission spectra of a QCL, we have calculated the optical spectra from Eq. (5) for the 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[7] ($m^*/m=0.042$ 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 purposes 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 the 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, σ_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 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 the allowed optical transition to the ground state. Eventually, with increasing B two peaks can be resolved and at $B\approx 2.2$ Tesla they have the same intensity. At a larger B the intensity of one of the peak will be suppressed and the optical spectrum again acquires a single-peak structure.

With an increasing magnetic field, the Zeeman energy becomes stronger and only the states with negative spin are occupied. As a result, there is only a single peak. This peak will be initially blue-shifted by an amount ~ 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.[8]

The condition $\alpha_u=-\alpha_l$ results in the strongest separation between two peaks. For a smaller difference between α_u and α_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 a decreasing difference between α_u and α_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 than the separation between them. The inset in Fig. 2 illustrates schematically the structure of two wells that gives the corresponding relation between the SO coupling, where the upper and lower states are localized in different wells.

Following the scheme for the formation of the double peak structure illustrated in Fig. 1 and taking into account the energy dispersion law [Eq. (2)], we can derive approximately the expression for the separation $\Delta\omega$ between the peaks

$$\hbar\,\Delta\omega = 2(\alpha_u-\alpha_l)(z_u-z_l)/l_B^2. \tag{6}$$

This approximate expression for $\Delta\omega$ does not depend on the Zeeman term, although the exact expression will have a weak dependence. The main effect of the Zeeman term is in the relative intensity of the two peaks. It always suppresses one of the peaks and enhances the other, so the double peak structure can exist only within a finite interval of the magnetic field. As can be seen from Eq. (6), to make the peaks well separated, we need to increase the difference $(\alpha_u-\alpha_l)$. The strongest effect should be expected when α in different wells have a different sign. The tuning of α can be done by a special arrangement of quantum wells and heterostructures.[12]

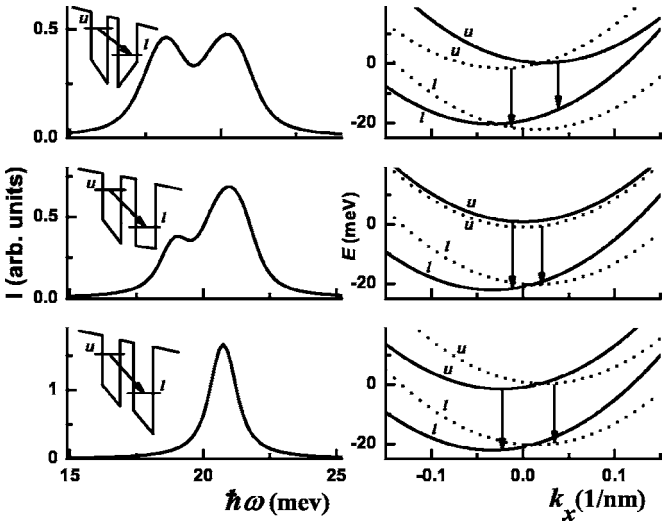

FIG. 2. Emission spectra for different structure of the active region of QCL (left panel), which result in different values of SO coupling in upper and lower subbands: (a) $\alpha_l=-\alpha_u=45$ meV nm, (b) $\alpha_u=0$ and $\alpha_l=45$ meV nm, (c) $\alpha_l=\alpha_u=45$ meV nm. The schematic illustration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

In Fig. 3, the evolution of a two-peak structure of the emission spectra with the change of the 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 α_u. With decreasing α_u, the separation between the peaks decreases and finally at small values of α_u two peaks could not be resolved.

To summarize, the main question that we have addressed in this paper is as follows: what is the possible manifestation of the SO interaction in the optical spectra of a QC structure

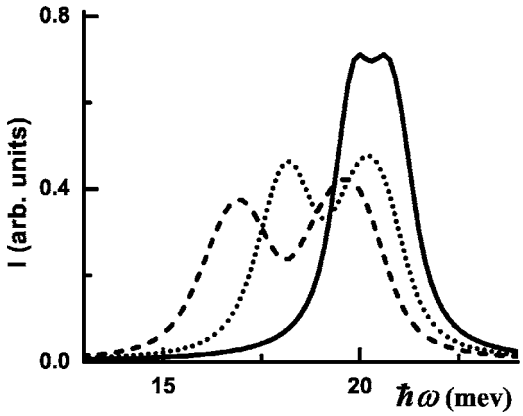

FIG. 3. Emission spectra for different values of α_u and the magnetic field under the condition $\alpha_l=-\alpha_u$; $\alpha_u=20$ meV nm and $B=0.8$ Tesla (solid line), $\alpha_u=45$ meV nm and $B=2.2$ Tesla (dotted line), and $\alpha_u=60$ meV nm and $B=3.24$ Tesla (dashed line).

and if it is possible to observe the SO splitting in the optical spectra. To allow transitions between different spin branches, we have introduced a parallel magnetic field. We have taken into account the shift of the dispersion relation in the k space due to the applied field. The modification of the subband energy levels due to this field is ignored, because this will only introduce some quantitative corrections, namely, corrections to the position and intensity of the double peak structure. As we have looked at the double-peak structure for relatively small magnetic fields, this approximation is well justified.

We have shown that in order to observe a double-peak structure, the quantum wells constituting the active region of a QCL should be asymmetric and optical transitions should be diagonal. The next important condition is that the SO couplings in different quantum wells should be very different. Then a two-peak emission line can develop within a certain interval of the parallel magnetic field. This interval is determined by the interplay of the Zeeman and SO terms in the Hamiltonian (1), where the Zeeman term always suppresses the two-peak structure. In our calculations we have used the g factor of the bulk material, $g=-14$. In quantum wells, the g factor can, in fact, be strongly suppressed,[13,14] which should make it easier to observe the two-peak structure due to the SO coupling in real systems. Since in a parallel magnetic field the occupation of the upper subband determines 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. We did not take into account the effective mass nonparabolicity in Eq. (1). This effect is very weak for electrons within a single subband due the small electron density. The nonparabolicity will only modify the effective electron mass in the different subbands. Since the peak separation [Eq. (6)] does not depend explicitly on the effective mass the nonparabolicy will have a rather weak effect on the two-peak structure.

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