Influence of the spin-orbit coupling on hole states in [001]- and [111]-oriented quantum dots of various geometry

Krzysztof Gawarek and Mateusz Krzykowski
Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Technology, Wybrzeże Wyspińskiego 27, 50-370 Wrocław, Poland

We study the influence of spin-orbit coupling on the hole spectrum in InAs/GaAs quantum dots grown on [001]- and [111]-oriented substrates belonging to symmetry point groups: $C_{2v}$, $C_{3v}$, and $D_{2d}$. We identify the irreducible representations linked to the states and discuss the selection rules, which govern the avoided-crossing pattern in magnetic-field dependence of the energy levels. We investigate the impact of various spin-orbit mechanisms on the strength of coupling between $s$- and $p$-shell states, which is a significant spin-flip channel in quantum dots. We show that dominant contribution to the coupling between some of these states comes from the shear strain. On the other hand, we demonstrate no coupling between $s$- and $p$-shell states in the [111]-oriented structure. The magnetic-field dependence of the hole states is calculated using 8-band $k\cdot p$ model and compared to the 14-band approach. We show a good agreement between these methods. Finally, we fit the simulation results by an effective model with empirical parameters.

I. INTRODUCTION

The properties of nanostructures related to the spin degree of freedom are interesting from the point of view of possible application in quantum information processing and spintronics. Coupling of spin to orbital degrees of freedom via the spin-orbit coupling (SOC) influences the carrier spectrum and could provide a channel of quantum coherent spin control. On the other hand, it may mix spin configurations, which leads to spin relaxation and dephasing processes. The lack of inversion symmetry, on the level of crystal lattice (bulk inversion asymmetry, BIA), in the shape of a nanostructure, or induced by external electric field (structure inversion asymmetry, SIA) gives rise to Dresselhaus and Rashba spin-orbit coupling, respectively. Furthermore, recent investigations show hidden spin polarization in centrosymmetric crystals.

Dresselhaus and/or Rashba interactions are commonly accounted for theoretically within effective models. While the parameters are available and well established for bulk materials, in the case of nanostructures the coupling strength is determined by their shape, composition profile, substrate orientation, strain and abrupt material interfaces. In consequence, a reliable quantitative description of the SIA effects requires advanced modeling. The impact of Dresselhaus and Rashba couplings on carrier states in a quantum dot (QD) were studied in various approaches. In the case of gate-defined quantum dots, the admixture mechanism coming from the coupling between $s$- and $p$-type states is a dominant spin-flip transition channel. It has been also shown that orientation of the magnetic field with respect to crystallographic axes strongly affects spin relaxation time in InAs/GaAs QDs, which was attributed to the interplay of Rashba and Dresselhaus couplings. This was addressed theoretically for [001]- and [111]-grown GaAs cuboidal QDs. In the case of InAs/GaAs self-assembled QDs, the influence of spin-orbit coupling is more complicated due to the presence of interfaces abrupt and symmetry-breaking shear strain. The latter gives spin admixture leading to electron spin relaxation, and this is one of the most important factors determining the splitting between hole $p$-type states. Symmetry of the self-assembled QD plays crucial role for its optical properties and exchange interaction. It has been also shown that the coupling between $s$- and $p$-shell electron states related to the Rashba interaction is enhanced by the dot anisotropy. Furthermore, the symmetry determines anticrossing pattern as well as affects spin mixing and relaxation in a double QD system. The properties of the nanostructure depends not only on its geometrical shape but also orientation of the underlying substrate. Due to potential application for entangled photon pairs generation, [111]-oriented QDs were subject of many theoretical and experimental works. It has been also demonstrated, that hole spin in [111]-oriented double QDs can be electrically controlled.

In this work, we investigate the influence of various mechanisms (Dresselhaus and Rashba interaction, shear strain) on the coupling between the $s$- and $p$-shell hole states in InAs/GaAs QDs. Within the 8-band $k\cdot p$ model, we calculate the magnetic-field dependence of the energy levels and study the width of avoided crossing between the $s$- and $p$-type state. We take into account [001]- and [111]-oriented substrates and consider three types of QDs representing $C_{2v}$, $C_{3v}$ and $D_{2d}$ symmetry point groups. For these, we identify the irreducible representations of hole states, discuss the selection rules, and demonstrate the absence of coupling between $s$ and both $p$-shell states for the [111]-oriented structure. We also show a good agreement between 8- and 14-band $k\cdot p$ approach. Additionally, for [001]-oriented lens shaped QD, we fit an effective model with empirical parameters to the numerical data.

The paper is organized as follows. In Sec. the methods used to calculate the strain distribution and the carrier states are described. In Sec. we present the results of numerical simulations for all of the considered
by perturbative elements explicitly added to $H_{6\text{D}}$ and $H_{6\text{C}}$ (see $H^{(D)}$ in the Appendix in Ref. [18]). The Dresselhaus SOC Hamiltonian for the electron (in 2-band $k \cdot p$ model) can be approximated by $H^{(D)}_{6\text{D}} \propto \langle k_z^2 \rangle (k_+ \sigma_+ + k_- \sigma_-)$, where $k_\pm = k_x \pm i k_y$, and $\sigma_\pm$ is the spin ladder operator. This couples $|M_z \approx 0, \uparrow \rangle$ to $|M_z \approx 1, \uparrow \rangle$ and $|M_z \approx 0, \uparrow \rangle$ to $|M_z \approx -1, \downarrow \rangle$, where $M_z$ denotes envelope angular momentum and $\uparrow, \downarrow$ refers to the spin orientation. In contrast, the Rashba coupling approximated by $H^{(R)}_{6\text{C}} \propto i (k_+ \sigma_- - k_- \sigma_+)$ connects $|M_z \approx 0, \uparrow \rangle$ to $|M_z \approx 1, \downarrow \rangle$, and $|M_z \approx 0, \downarrow \rangle$ to $|M_z \approx -1, \uparrow \rangle$. On the other hand, the influence of the spin-orbit interaction for holes is much more complicated compared to the electron[12]. In this case, the Rashba coupling may mix $|M_z \approx 0, \uparrow \rangle$ to both $|M_z \approx 1, \downarrow \rangle$ and $|M_z \approx -1, \downarrow \rangle$ (and vice-versa), where $\uparrow, \downarrow$ refers to band angular momentum (see Appendix B).

III. NUMERICAL RESULTS AND SYMMETRY CLASSIFICATION

A. [001]-oriented lens shaped QD

We calculated the magnetic-field dependence of the lowest-energy hole states in the lens-shaped QD. The shape of such a structure does not have the inversion symmetry. The energy levels obtained from 8-band $k \cdot p$ simulations are presented in Fig. 2. The two lowest-energy states (marked by the red lines) exhibit s-type symmetry, their average value of the axial projection of envelope angular momentum $\langle M_z \rangle$ is close to 0. The next four states (plotted with green lines) exhibit p-type symmetry with $\langle M_z \rangle \approx \pm 1$. Although the shape of the QD transforms according to the $C_{\infty v}$ group, the underlying crystal lattice limits the symmetry of the system to the $C_{2v}$ (at $B = 0$ T). Due to the spin-orbit coupling, the system must be described in terms of the double group representation[40,42]. The symmetry point group $C_{2v}$ contains only one irreducible double group representation $D_{1/2}$ (see the character table in Appendix A) and all states must belong to it. Since $D_{1/2}$ is two-dimensional, the states are doubly degenerate (which in fact results from the time-reversal symmetry). At nonzero axial magnetic field $B \neq 0$, the symmetry of the system is further reduced to $C_{111/2}$. In this case, $D_{1/2}$ splits into two one-dimensional representations: $D_A$ and $D_B$, where $D_A = D^*_B$ (see Tab. 11 in Appendix A). For each state $|\Psi\rangle$ we found the relevant irreducible representation $\alpha$ via projection $\hat{P}^{(\alpha)}|\Psi\rangle$, where $\hat{P}^{(\alpha)} = \sum_i \chi^*(\hat{R}_i)\hat{R}_i$, and $\chi(\hat{R}_i)$ is the character of the representation $\alpha$ for the symmetry operation $\hat{R}_i$. The states $s_1$, $p_2$, and $p_3$ belong to $D_A$, whereas $s_2$, $p_1$, and $p_4$ to $D_B$. According to the selection rules, two states can couple if they belong to the same irreducible representation. In the presence of SOC, an avoided crossing pattern appears in the system spectrum. In the considered system, the spin-orbit cou-
FIG. 2. (Color online) Magnetic-field dependence of the lowest hole energy levels for the lens shaped [001]-oriented QD. The inset contains enlarged part of the plot with anticrossing between s- and p-type states. Energy $E = 0$ refers to the unstrained GaAs valence-band edge.

pling in the hole $p$ shell favors the parallel orientation of the envelope and band angular momenta (see a detailed discussion in Ref. [18]). At $B \approx 9$ T, there is an avoided crossing between $p_2$ and $p_3$ (region A in Fig. 2), they have the same orientation of the band angular momenta but different $M_z$. Furthermore, an avoided crossing appears between states $s_2$ ($\langle M_z \rangle \approx 0, \downarrow$) and $p_1$ ($\langle M_z \rangle \approx 1, \uparrow$) at region B, where its width is $\Delta E_{sp} = 0.246$ meV.

To assess the importance of various SOC mechanisms and check the accuracy of 8-band $k \cdot p$, we compared the value of $\Delta E_{sp}$ obtained within several degrees of approximation. As shown in Table I, the results from 8- and 14-band $k \cdot p$ are in a good agreement. Dresselhaus terms are negligible for $\Delta E_{sp}$, however they could be important for $s_1 - p_3$ and $s_2 - p_4$ couplings (which is hard to estimate, because it is not represented by any avoided crossing in the considered spectrum). In the last approach, the influence of shear strain in the valence band is neglected by setting the deformation potential $d_v = 0$. In this case, $\Delta E_{sp}$ is significantly reduced, which suggest that the shear strain is one of the most important factors determining the $s - p$ coupling.

The Rashba coupling can rise due to external potentials. We calculated $\Delta E_{sp}$ at the axial electric field $F = 30$ kV/cm and obtained $\Delta E_{sp} = 0.243$ meV, while opposite direction $F = -30$ kV/cm led to $\Delta E_{sp} = 0.248$ meV.

| Model | $\Delta E_{sp}$ (meV) |
|-------|----------------------|
| 14-band $k \cdot p$, full | 0.25481 |
| 8-band $k \cdot p$, full | 0.24627 |
| 8-band $k \cdot p$, Dresselhaus terms $H^{(D)} = 0$ neglected | 0.24565 |
| 8-band $k \cdot p$, shear strain neglected ($d_v = 0$) | 0.11679 |

This shows, that for the considered QD the axial electric field generates the Rashba coupling, which is much weaker than the structure inversion asymmetry resulting from the QD shape.

B. [001]-oriented disk shaped QD

The magnetic-field dependence of energy levels calculated for the [001]-oriented disk-shaped QD is presented in Fig. 3. For such a system, at $B = 0$, the symmetry point group is $D_{2d}$. According to the character table (Tab. IV in Appendix A), there are two irreducible double-group representations $D_{1/2}$ and $D'$. In the presence of magnetic field, the symmetry of the system is...
C. [111]-oriented lens shaped QD

Finally, we investigate the magnetic-field dependence for a lens-shaped QD grown in the [111] direction. The simulation results are presented in Fig. 4. At $B = 0$, the symmetry of the system is $C_{3v}$, while the axial magnetic field (now oriented along the [111] direction) reduces it to $C_{3}$ (see character tables in Appendix A). This leads to different selection rules compared to the cases considered previously. We identified the representations of the states: $s_1$ and $s_2$ belong to $D_{1}$, $p_1$ and $p_2$ to $D_{II}$, $p_3$ to $D_{IV}$, and $p_4$ to $D_{III}$ representation. Since $s_2$ and $p_3$ states belong to different representations, there is no avoided crossing between their energy levels. For the same reason, we obtain a crossing between $p_2$ and $p_3$ at about 3 T. In contrast to the lens-shaped QD, at weak magnetic field, the states with antiparallel envelope and band angular momenta have lower energy compared to the opposite configuration.

The symmetry of the system can be further reduced by external electric field. For axial field, the symmetry changes from $D_{2d}$ to $C_{2v}$ (and from $S_4$ to $C_2$ at $B \neq 0$). In this case, the Rashba coupling between upper $s$-shell state ($M_z \approx 0, \downarrow$) and the $p$-shell state ($M_z \approx 1, \uparrow$) appears. The simulation results are presented in the inset of Fig. 3. The width of the anticrossing increases linearly with the electric field, and at $F = 0$ there is a crossing between the relevant energy levels.

FIG. 3. (Color online) Magnetic-field dependence of the lowest hole energy levels for the disk shaped [001]-oriented QD. The inset contains the avoided crossing width between $s$- and $p$-shell energy levels as a function of external axial electric field $F$.

FIG. 4. (Color online) Magnetic field dependence of the lowest hole energy levels for the lens shaped [111]-oriented QD.
small anticrossings in the simulation results are numerical artifacts related to the discretization on a rectangular mesh. In contrast to the [001]-oriented disk-shaped QD, the crossing between \( s_2 \) and \( p_1 \) energy branches can not be resolved by the axial electric field because it does not change the symmetry of the system.

IV. CONCLUSIONS

We have investigated the hole \( s-p \) coupling related to the spin-orbit interaction for three QDs representing symmetry point groups: \( C_{2v}, C_{3v} \) and \( D_{2d} \). We have shown that in the case of [001]-oriented lens shaped QD important contribution to the width of the avoided crossing between \( s- \) and \( p- \) shell energies comes from the shear strain. We have compared the results from 8- and 14-band \( k \cdot p \) models and have obtained a good agreement between these methods. For [001]-oriented lens-shaped QD, we have also calculated the Rashba effect resulting from the external axial electric field, and demonstrated a very small change in the anticrossing width compared to the spin-orbit interaction for three QDs representing a very small change in the anticrossing width compared from the external axial electric field, and demonstrated no coupling between \( s- \) and \( p- \) shell states in the [111]-oriented lens shaped QD.

ACKNOWLEDGMENTS

This work was supported by the Polish National Science Centre (via Grant No. 2014/13/B/ST3/04603). Calculations have been carried out using resources provided by Wroclaw Centre for Networking and Supercomputing (http://wcssp.pl), Grant No. 203. We would like to thank Paweł Machniński and Michal Gawelczyk for their helpful suggestions. We are also grateful to Michal Gawelczyk for sharing his implementation of the blur algorithm.

Appendix A: Symmetry point groups

In this Appendix we present the character tables of the symmetry point groups \( C_{2v}, C_2, C_{3v}, C_3, D_{2d} \) and \( S_4 \). In the presence of spin, the double group representations are used. Here \( \mathcal{R} \) denotes the rotation of \( 2\pi \), while the neutral element \( \mathcal{E} \) corresponds to the rotation of \( 4\pi \). In the group \( C_{2v} \), the two-dimensional irreducible representation \( D_{1/2} \) contains diagonal matrices \( \Gamma^{(D_{1/2})(E)} \), \( \Gamma^{(D_{1/2})(\mathcal{R})} \), \( \Gamma^{(D_{1/2})(C_2)} \), but the matrices representing reflections \( \sigma_v \) have off-diagonal elements. Hence, the reduction \( C_{2v} \) to subgroup \( C_2 \) leaves all \( D_{1/2} \) non-diagonal matrices. In consequence it can be separated into two irreducible representations \( D_A, D_B \).

Within the 8-band \( k \cdot p \) model with envelope function approximation, the eigenstates of the system have a form

\[
|\Psi_n\rangle = \sum_{m=1}^{8} \Phi_{n,m}(r) |J, J_z\rangle_m,
\]

where \( \Phi_{n,m} \) is the envelope and \( |J, J_z\rangle_m \) describes the Bloch part (at \( k = 0 \)) with the total band angular momentum \( J \) and its axial projection \( J_z \). The basis contains: conduction band \( |\frac{1}{2}, \pm\frac{1}{2}\rangle_c \), heavy-hole \( |\frac{3}{2}, \pm\frac{1}{2}\rangle_h \), light-hole \( |\frac{3}{2}, \pm\frac{1}{2}\rangle_l \), and two split-off subbands \( |\frac{1}{2}, \pm\frac{1}{2}\rangle_v \). To find the irreducible representation of a given state \( |\Psi_n\rangle \), we performed the projection with operator \( \mathcal{P}(\alpha) = \sum_i \chi^*(\hat{R}_i)\hat{R}_i \), where \( \chi(\hat{R}_i) \) is a character of the representation \( \alpha \) for the symmetry operation \( \hat{R}_i \). As the envelope part changes slowly in scale of the unit cell, we act with \( \hat{R}_i \) on the envelope and Bloch part of the wave functions separately, e.g., the effect of axial rotation \( C_k \) is \( C_k \Phi_{n,m}(r) = \Phi_{n,m}(C_k^{-1}r) \), and \( C_k |J, J_z\rangle = e^{-iJz2\pi/k} |J, J_z\rangle \). We express the improper rotations \( S_k \) as \( S_k \equiv \sigma_h C_k = \mathcal{I}C_k\mathcal{I}_Z \), where \( \sigma_h \) is reflection in plane perpendicular to the rotation axis and \( \mathcal{I} \) is the inversion operator. The effect of inversion is \( |\frac{1}{2}, \pm\frac{1}{2}\rangle_c = |\frac{1}{2}, \pm\frac{1}{2}\rangle_c \) for the conduction band, and \( |J, J_z\rangle_v = -|J, J_z\rangle_v \) for the valence-band basis states.

| \( C_{2v} \) | \( E \) | \( \mathcal{R} \) | \( C_2 \) | \( \sigma_v(xz) \) | \( \sigma_v(yz) \) | \( \sigma_v(z) \) |
|---|---|---|---|---|---|
| \( A_1 \) | 1 | 1 | 1 | 1 | 1 |
| \( A_2 \) | 1 | 1 | 1 | -1 | -1 |
| \( B_1 \) | 1 | 1 | -1 | 1 | -1 |
| \( B_2 \) | 1 | 1 | -1 | 1 | -1 |
| \( D_{1/2} \) | 2 | -2 | 0 | 0 | 0 |

| \( C_2 \) | \( E \) | \( C_2 \) | \( \mathcal{R} \) | \( \mathcal{R}C_2 \) |
|---|---|---|---|
| \( A_1 \) | 1 | 1 | 1 | 1 |
| \( A_2 \) | 1 | -1 | 1 | -1 |
| \( B_1 \) | 1 | -1 | 1 | -1 |
| \( D_A \) | 1 | i | -i | -i |
| \( D_B \) | 1 | -i | i | i |

Appendix B: Effective model

In this part we describe the effective model that can be used to interpret the simulation results. We utilize the Fock-Darwin model supplemented by additional terms representing system anisotropy as well as the spin-orbit interaction.

In the axial approximation, the states in a QD can be characterized according to their axial projection of the
TABLE IV. Character table of $D_{2d}$ symmetry double point group[13]

| $D_{2d}$ | $E$ | $R$ | $2S_4$ | $2RS_4$ | $C_2$ | $RC_2$ | $2C'_2$ | $2RC'_2$ | $2R\sigma_d$ |
|---------|-----|-----|--------|--------|-------|--------|--------|--------|--------|
| $A_1$   | 1   | 1   | 1      | 1      | 1     | 1      | 1      | 1      | 1      |
| $B_1$   | 1   | -1  | -1     | 1      | 1     | -1     | -1     | -1     | -1     |
| $B_2$   | 1   | 1   | -1     | -1     | 1     | -1     | -1     | -1     | -1     |
| $E$     | 2   | -2  | 0      | -2     | 0     | 0      | 0      | 0      | 0      |

$D_{1/2}$ | 2 | -2 | $\sqrt{2}$ | $-\sqrt{2}$ | 0 | 0 | 0 | 0 |

$D'$ | 2 | -2 | $-\sqrt{2}$ | $\sqrt{2}$ | 0 | 0 | 0 | 0 |

TABLE V. Character table of $S_4$ symmetry double point group[13]

| $S_4$  | $E$ | $S_4$ | $C_2$ | $R$ | $RS_4$ | $RC_2$ | $RS_4^2$ |
|--------|-----|-------|-------|-----|--------|--------|----------|
| $A$    | 1   | 1     | 1     | 1   | 1      | 1      | 1        |
| $B$    | 1   | -1    | -1    | 1   | -1     | 1      | -1       |
| $E_1$  | 1   | $i$   | -1    | $i$ | 1      | -1     | $i$      |
| $E_2$  | 1   | $i$   | 1     | -1  | $i$    | $i$    | 1        |

$D_1$ | 1 | $-\frac{1+i}{\sqrt{2}}$ | $-\frac{1+i}{\sqrt{2}}$ | $\frac{1-i}{\sqrt{2}}$ | $i$ | $\frac{1-i}{\sqrt{2}}$ | $i$ | $\frac{1-i}{\sqrt{2}}$ |

$D_{II}$ | 1 | $\frac{1-i}{\sqrt{2}}$ | $\frac{1-i}{\sqrt{2}}$ | $-\frac{1+i}{\sqrt{2}}$ | $-i$ | $\frac{1+i}{\sqrt{2}}$ | $-i$ | $\frac{1+i}{\sqrt{2}}$ |

$D_{II}$ | 1 | $\frac{1-i}{\sqrt{2}}$ | $\frac{1-i}{\sqrt{2}}$ | $-\frac{1+i}{\sqrt{2}}$ | $i$ | $\frac{1+i}{\sqrt{2}}$ | $i$ | $\frac{1+i}{\sqrt{2}}$ |

$D_{IV}$ | 1 | $\frac{1+i}{\sqrt{2}}$ | $\frac{1+i}{\sqrt{2}}$ | $-\frac{1-i}{\sqrt{2}}$ | $-i$ | $\frac{1-i}{\sqrt{2}}$ | $-i$ | $\frac{1-i}{\sqrt{2}}$ |

TABLE VI. Character table of $C_{3v}$ symmetry double point group[13]

| $C_{3v}$ | $E$ | $R$ | $2C'_{3a}$ | $2RC'_{3a}$ | $3\sigma_v$ | $3R\sigma_v$ |
|----------|-----|-----|-----------|-------------|-------------|-------------|
| $A_1$    | 1   | 1   | 1         | 1           | 1           | 1           |
| $A_2$    | 1   | 1   | 1         | 1           | 1           | 1           |
| $E$      | 2   | -2  | -1        | 0           | 0           | 0           |

$D_{1/2}$ | 2 | -2 | -1 | 0 | 0 |

$D'$ | 1 | -1 | -1 | 1 | i | -i |

$D''$ | 1 | -1 | -1 | 1 | -i | i |

TABLE VII. Character table of $C_{3v}$ symmetry double point group[13]

| $C_{3v}$ | $E$ | $C_3$ | $C^2_3$ | $R$ | $RC_3$ | $RC^2_3$ |
|----------|-----|-------|--------|-----|--------|--------|
| $A_1$    | 1   | 1     | 1      | 1   | 1      | 1      |
| $B_1$    | 1   | $e^{2\pi i/3}$ | $e^{4\pi i/3}$ | 1 | $e^{2\pi i/3}$ | $e^{4\pi i/3}$ |
| $B_2$    | 1   | $-e^{2\pi i/3}$ | $e^{4\pi i/3}$ | 1 | $-e^{2\pi i/3}$ | $e^{4\pi i/3}$ |

$D_1$ | 1 | $-1$ | 1 | 1 | -1 | -1 |

$D_{II}$ | 1 | $e^{2\pi i/3}$ | $e^{4\pi i/3}$ | -1 | $e^{2\pi i/3}$ | $-e^{4\pi i/3}$ |

$D_{III}$ | 1 | $-e^{2\pi i/3}$ | $e^{4\pi i/3}$ | -1 | $-e^{2\pi i/3}$ | $-e^{4\pi i/3}$ |

The envelope angular momentum $M_z$, where the $s$ shell contains states with $M_z = 0$ and the $p$ shell with $M_z = \pm 1$. In fact, $p$-type states can be mixed due to anisotropy related to the piezoelectric potential, dot elongation and other possible effects. Due to the dominant heavy-hole components of the considered states, their axial projections of band angular momenta ($\uparrow, \downarrow$) can be approximated by $(J_z) \approx \pm \frac{3}{2}$. Furthermore, the spin-orbit coupling distinguishes the mutual alignment of the envelope and the band angular momenta as well as it can mix $s$- and the $p$-shell states. We express the Hamiltonian in the basis $|M_z J_z\rangle = |M_z\rangle \otimes |J_z\rangle$ and consider $s$ and $p$ shells {\( |0 \uparrow\rangle, |1 \uparrow\rangle, |1 \downarrow\rangle\), {\( |0 \downarrow\rangle, |1 \downarrow\rangle\)}}. The effective Hamiltonian reads

\[
H_{\text{eff}} = E_s |0\rangle\langle 0| \otimes I_2 + E_p (|1\uparrow\rangle\langle 1\uparrow| + |1\downarrow\rangle\langle 1\downarrow|) \otimes I_2 + V_a (|\downarrow\rangle\langle \uparrow| + |\uparrow\rangle\langle \downarrow|) \otimes I_2 \nonumber
\]

\[+\frac{1}{2} \mu_B [g_s |0\rangle\langle 0| + g_p (|1\uparrow\rangle\langle 1\uparrow| + |1\downarrow\rangle\langle 1\downarrow|)] B_z \otimes \sigma_z \nonumber\]

\[+ \frac{1}{2\hbar} V'_{sp} L_z \otimes \sigma_z \nonumber\]

\[+ V'_{sp} (|0\rangle\langle -1| \otimes |\uparrow\rangle\langle \uparrow| + |1\rangle\langle 0| \otimes |\downarrow\rangle\langle \downarrow|) \nonumber\]

\[- V'_{sp} (|0\rangle\langle 1| \otimes |\downarrow\rangle\langle \downarrow| + |1\rangle\langle 0| \otimes |\uparrow\rangle\langle \uparrow|) \nonumber\]

\[+ \alpha_s B_z^2 \langle 0| \otimes I_2 \nonumber\]

\[+ \alpha_p B_z^2 \langle 1\uparrow\rangle\langle 1\uparrow| + |1\downarrow\rangle\langle 1\downarrow| \otimes I_2, \nonumber\]

where $E_s$, $E_p$ are the bare energies ($B = 0$, axial approximation, SOC neglected) of the $s$- and $p$-type states respectively, $I_2$ is the unit operator in the band angular momentum formal subsystem, $V_a$ is a parameter accounting for the anisotropy, $L_z$ is the operator of the $z$ component of the envelope angular momentum, $g_s$ and $g_p$ are $g$-factors in $s$- and $p$-shell respectively, $\sigma$ are the Pauli matrices, $V'_{sp}$ describes the spin-orbit coupling for the $p$-states, $V'_{sp}$ is a parameter related to the coupling between $s$ and $p$ states, finally $\alpha_s$ and $\alpha_p$ account for the diamagnetic shift. We neglect the coupling of $|0 \uparrow\rangle$ to $|1 \downarrow\rangle$, and $|0 \downarrow\rangle$ to $|1 \uparrow\rangle$ because they are not represented by any avoided crossing in the considered spectrum. The effective Hamiltonian can be then written in matrix block form

\[
H_{\text{eff}} = \left( \begin{array}{ccc}
H_{\text{env}} + \frac{1}{2} H_1 & \frac{1}{2} H_1 & H_2 \\
\frac{1}{2} H_1 & H_{\text{env}} & \frac{1}{2} H_1 \\
H_2 & \frac{1}{2} H_1 & H_{\text{env}} - \frac{1}{2} H_1
\end{array} \right),
\]

where

\[
H_{\text{env}} = \begin{pmatrix}
E_s & 0 & 0 \\
0 & E_p + W B_z & V_a \\
0 & V_a & -E_p - W B_z
\end{pmatrix}
\]

\[
H_1 = \begin{pmatrix}
\mu_B g_s B_z & 0 & 0 \\
0 & \alpha_p B_z^2 & 0 \\
0 & 0 & \alpha_p B_z^2
\end{pmatrix}
\]

\[
H_2 = \begin{pmatrix}
0 & V'_{sp} & 0 \\
0 & 0 & V'_{sp} \\
0 & 0 & 0
\end{pmatrix}
\]
We fitted the simulation data from Fig. 2 with the effective model and obtained the following parameters: $E_a = -229.14$ meV, $E_p = -203.75$ meV, $V_a = 0.33328$ meV, $W = -0.46764$ meV/T, $g_s = -5.5745$, $g_p = -0.11141$, $V_{sp}^{(so)} = -8.0707$ meV, $V_{pp}^{(so)} = 123.13$ μeV, $\alpha_s = 3.0834$ μeV/T², and $\alpha_p = 5.0050$ μeV/T². Such parameter set gives energies in a good agreement with these obtained from the 8-band $k\cdot p$ model.

[1] Krzysztof.Gawarecki@pwr.edu.pl

1. Zutić, J. Fabian, and S. D. Sarma, Rev. Mod. Phys. 76, 323 (2004).
2. R. Hanson, L. P. Kouwenhoven, J. R. Petta, S. Tarucha, and L. M. Vandersypen, Rev. Mod. Phys. 79, 1217 (2007).
3. D. Loss and D. P. DiVincenzo, Phys. Rev. A 57, 120 (1998).
4. E. Y. S. Joe, Spintronics in Nanoscale Devices (Pan Stanford Publishing, 2013).
5. C. Flindt, A. S. Sørensen, and K. Flensberg, Phys. Rev. Lett. 97, 240501 (2006).
6. A. V. Khaetskii and Y. V. Nazarov, Phys. Rev. B 61, 12639 (2000).
7. A. V. Khaetskii and Y. V. Nazarov, Phys. Rev. B 64, 125316 (2001).
8. V. N. Golovach, A. Khaetskii, and D. Loss, Phys. Rev. B 77, 045328 (2008).
9. J. I. Climente, C. Segarra, and J. Planelles, New J. Phys. 15, 093009 (2013).
10. A. Mielnik-Pyszczorski, K. Gawarecki, M. Gawelczyk, and P. Machnikowski, Phys. Rev. B 97, 245313 (2018).
11. C. Segarra, J. I. Climente, F. Rajadell, and J. Planelles, J. Phys. Condens. Matter 27, 415301 (2015).
12. R. Winkler, Spin-Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems (Springer, 2003).
13. X. Zhang, Q. Liu, J.-W. Luo, A. J. Freeman, and A. Zunger, Nat. Phys. 10, 387 (2014).
14. D. V. Bulaev and D. Loss, Phys. Rev. B 71, 205324 (2005).
15. S. Avetisyan, P. Pietiläinen, and T. Chakraborty, Phys. Rev. B 85, 153301 (2012).
16. S. Avetisyan, P. Pietiläinen, and T. Chakraborty, Phys. Rev. B 86, 205301 (2013).
17. A. Manaselbyan and T. Chakraborty, Eur. Phys. Lett. 88, 17003 (2009).
18. K. Gawarecki, Phys. Rev. B 97, 235408 (2018).
19. P. Scarlino, E. Kawakami, P. Stano, M. Shafiie, C. Reichl, W. Wegscheider, and L. Vandersypen, Phys. Rev. Lett. 113, 256802 (2014).
20. C. Segarra, J. Planelles, J. I. Climente, and F. Rajadell, New J. Phys. 17, 033014 (2015).
21. A. Mielnik-Pyszczorski, K. Gawarecki, M. Gawelczyk, and P. Machnikowski, Phys. Rev. B 97, 1 (2018).
22. M. Zieliński, Y. Don, and D. Gershoni, Phys. Rev. B 91, 085403 (2015).
23. Multi-Band Effective Mass Approximations, Vol. 94 of Lecture Notes in Computational Science and Engineering, edited by M. Ehrhardt and T. Koprucu (Springer International Publishing, 2014).
24. M. F. Doty, J. I. Climente, A. Greilich, M. Yakes, A. S. Bracker, and D. Gammon, Phys. Rev. B 81, 035308 (2010).
25. J. M. Daniels, P. Machnikowski, and T. Kuhn, Phys. Rev. B 88, 205307 (2013).
26. P.-L. Ardelt, K. Gawarecki, K. Müller, A. Waebler, A. Bechtold, K. Oberhofer, J. Daniels, F. Klotz, M. Bichler, T. Kuhn, H. Krenner, P. Machnikowski, and J. Finley, Phys. Rev. Lett. 116, 077401 (2016).
27. X. Ma, G. W. Bryant, and M. F. Doty, Phys. Rev. B 93, 245402 (2016).
28. R. Singh and G. Bester, Phys. Rev. Lett. 103, 063601 (2009).
29. S. Schulz, S. Schumacher, and G. Czycholl, Eur. Phys. J. B 64, 51 (2008).
30. E. Stock, T. Warming, I. Ostapenko, S. Rodt, A. Schliwa, J. A. Töfllinger, A. Lochmann, A. I. Toropov, S. A. Moschenko, D. V. Dmitriev, V. A. Häisler, and D. Bimberg, Appl. Phys. Lett. 96, 093112 (2010).
31. T. Mano, M. Abbarchi, T. Kuroda, B. McSkimming, A. Oltake, K. Mitsuishi, and K. Sakoda, Appl. Phys. Express 3, 065203 (2010).
32. I. A. Ostapenko, E. Stock, T. Warming, S. Rodt, A. Schliwa, M. Öztürk, J. A. Töfllinger, A. Lochmann, D. Bimberg, A. I. Toropov, S. A. Moschenko, D. V. Dmitriev, and V. A. Häisler, J. Phys. Conf. Ser. 245, 012003 (2010).
33. S. Schulz, M. A. Caro, E. P. O’Reilly, and O. Marquardt, Phys. Rev. B 84, 125312 (2011).
34. O. Marquardt, E. P. O’Reilly, and S. Schulz, J. Phys. Condens. Matter 26, 035303 (2014).
35. M. Świderski and M. Zieliński, Phys. Rev. B 95, 125407 (2017).
36. C. Pryor, J. Kim, L. W. Wang, A. J. Williamson, and A. Zunger, J. Appl. Phys. 83, 2548 (1998).
37. G. Bester, X. Wu, D. Vanderbilt, and A. Zunger, Phys. Rev. Lett. 96, 187602 (2006).
38. M. A. Caro, S. Schulz, and E. P. O’Reilly, Phys. Rev. B 91, 075203 (2015).
39. T. Eisfeller, Ph.D. thesis, Technical University of Munich, 2012.
40. M. S. Dresselhaus, G. Dresselhaus, and A. A. Jorio, Group theory : application to the physics of condensed matter (Springer-Verlag, 2010).
41. P. Yu and M. Cardona, Fundamentals of semiconductors : physics and materials properties (Springer, 2010).
42. G. L. Bir and G. E. Pikus, Symmetry and strain-induced effects in semiconductors (Wiley, 1974).
43. L. Piel, Ideas of quantum chemistry (Elsevier, 2013), p. Appendix C.
44. C. J. C. J. Bradley and A. P. Cracknell, The mathematical theory of symmetry in solids : representation theory for point groups and space groups (Oxford, 1972).