Effect of the inter-subband spin-orbit interaction on the spin transistor operation

P. Wójcik and J. Adamowski
AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, al. Mickiewicza 30, Kraków, Poland

We consider the electron transport in the Datta-Das spin transistor within the two-subband model taking into account the intra- and inter-subband spin-orbit (SO) interaction and study the influence of the inter-subband SO coupling on the spin-transistor operation. Starting from the model, in which the SO coupling constants are treated as parameters, we show that the inter-subband SO interaction strongly affects the ordinary conductance oscillations predicted for the transistor with the single occupancy. Interestingly, we find that even in the absence of the intra-subband SO interaction, the conductance oscillates as a function of the inter-subband SO coupling constant. This phenomenon is explained as resulting from the inter-subband transition with spin-flip. Next, we consider the realistic spin transistor model based on the gated Al$_0.48$In$_{0.52}$As/Ga$_0.47$In$_{0.53}$As double quantum well, for which the SO coupling constants are determined by the Schrödinger-Poisson approach.

We show that the SO coupling constants rapidly change around $V_g = 0$, which is desirable for the spin transistor operation. We demonstrate that for high electron densities the inter-subband SO interaction starts to play the dominant role. The strong evidence of this interaction is the reduction of the conductance for gate voltage $V_g = 0$, which leads to the reduction of the on/off conductance ratio.

I. INTRODUCTION

The coherent manipulation of the electron spin in semiconductor materials via the coupling of the electron’s motion with its spin degree of freedom is a key ingredient in most spintronic devices.\cite{1} The special place among them belongs to the spin field effect transistor (spin-FET)\cite{2} in which the electrically tunable spin-orbit interaction of Rashba\cite{3} is used to control - via the spin rotation - the electric current between ferromagnetic source and drain. However, the experimental realization of the functional spin-FET encounters serious physical obstacles, i.e. the low efficiency of the spin injection from ferromagnet into semiconductor due to the resistance mismatch\cite{4} and the spin relaxation induced mostly by the Dyakonov-Perel mechanism.\cite{5} Both these effects lead to the low electrical signal and the low ratio of the ”on-conductance” to the ”off-conductance” in the first experimental realization of the spin-FET.\cite{6} Note, that the maximum value of the on/off conductance ratio defined as $G_{on}/G_{off} = (1 + P_S P_D)/(1 - P_S P_D)$, where $P_S (P_D)$ is the spin injection (detection) efficiency in the source (drain), has a value 2.92 for $P_S = P_D = 70\%$ (the highest spin injection efficiency reported at room temperature), which is insufficient for the electric circuit application. Therefore, the basic condition which has to be meet in the experimental setup of the spin-FET is the spin injection (detection) nearly equals to 100% - the ratio $G_{on}/G_{off} = 10^5$, adequate for the modern electronics, requires $P_S = P_D = 99.9995\%$.\cite{7} This requirement can be satisfied only by the use of the semiconductor spin filters such as magnetic resonant tunneling diodes\cite{8,9} or quantum point contacts (QPC) with the lateral Rashba SO interaction.\cite{10,11} The latter have been successfully used as the spin injector and detector in the recent experiment,\cite{12,13} in which about $10^5$ times greater conductance oscillations have been observed as compared to the conventional spin-FET based on ferromagnets.\cite{14} The further improvement of the spin transistor operation involves the suppression of the spin relaxation. For this purpose the layer conduction channel with two dimensional electron gas (2DEG) should be replaced by the nanowire\cite{15} in which the Dyakonov-Perel mechanism of the spin relaxation is strongly suppressed by the motional narrowing effect.\cite{16,17} Another concept assumes equating the Rashba and Dresselhaus terms\cite{18,19} which generates the persistent spin helix state with extraordinary long spin lifetime. Nevertheless, this concept\cite{20,21,22} of the spin transistor is still waiting for the experimental realization.

The alternative spin transistor design in which the spin signal is observed over the distance $50\,\mu$m has been recently demonstrated by Betthausen et al. in Ref. 23. In this design, the spin transistor action is generated by the Landau-Zener transitions, which occur in the combined homogeneous and helical magnetic fields. The latter is generated by the ferromagnetic stripes located above the conduction channel made of the magnetic semiconductor. As shown in Refs. 25 and 26, by keeping the transport in the adiabatic regime, the spin state is protected against the electron scattering on defects. The switching into the non-adiabatic regime generates the additional conductance dips, which result from the resonant Landau-Zener transitions.\cite{27} Although the alternative spin-FET\cite{28} seems to be characterized by the long spin lifetime, it requires the application of the external homogeneous magnetic field, which is difficult to be applied in the integrated circuit. For this reason, in our recent paper 28 we have proposed analogous design, in which the spin transistor action is generated by all-electric means with the use of the lateral Rashba SO interaction.

Most of the theoretical studies and experimental realizations of the spin transistor reported so far have...
been based on 2DEG fabricated in the narrow n-type AlInAs/GaInAs well. In the sufficiently narrow quantum well the electrons occupy only the first subband, i.e. we are dealing with the lowest-energy state occupancy. However, the recent interest of researchers is directed towards the systems with the wide and coupled quantum wells with double occupancy (two lowest-energy subbands are occupied), which leads to interesting physical effects such as band anticrossings or spin mixing. The SO interaction in 2DEG quantum well with two subbands has been studied by Bernardes et al. in Ref. 32. The inter-subband-induced SO interaction has been found which results from coupling between states with opposite parity. This inter-subband SO interaction, quadratic in the momentum, can give raise to interesting physical phenomena such as band anticrossings or spin mixing. All these new phenomena motivated us to investigate the spin-FET based on the conduction channel with double occupancy and analyze the influence of the inter-subband-induced SO interaction on the spin transistor operation.

In the present paper, we consider the electron transport in the Datta and Das spin transistor architecture within the two subband model, which allows us to include the intra- and inter-subband SO couplings. Starting from the model, in which the values of the SO coupling constants are treated as the parameters, we analyze the influence of the inter-subband-induced SO interaction on the conductance and answer the question how this type of SO interaction affects the operation of the spin transistor. Next, we consider the realistic double quantum well with the applied external gate voltages for different electron concentrations. Following the method proposed in Ref. 34, based on the $8 \times 8$ Kane model within the $k \cdot p$ approximation, we determine the intra- and inter-subband SO coupling constants via the self-consistent Schrödinger-Poisson procedure. These values are used in the conductance calculations performed by the scattering matrix method. We reproduce the resonant behavior of the SO coupling constants reported for a double quantum well. This resonant behavior for which the values of the SO parameters change abruptly near the zero gate voltage is suitable for the spin transistor application in which the on/off transition should be realized in the narrow voltage range. By calculating the conductance for different gate voltages, we analyze the spin transistor operation for different electron concentrations $n_e$ and find that for high $n_e$ the inter-subband-induced SO interaction start to play a crucial role leading to the suppression of the on/off conductance ratio. Finally, the spin transistor operation is analyzed in the context of the coupling between the quantum wells which is determined by the width of the central barrier.

The paper is organized as follows: in section II we introduce the model of the nanostructure and briefly review the Kane Hamiltonian, which leads to the formulas for the intra- and inter-subband SO coupling constants. Next, we describe the self-consistent Schrödinger-Poisson method used to the SO coupling constants calculations. Finally, we derive the $4 \times 4$ Hamiltonian in two subband model used to the electronic transport calculations within the scattering matrix approach. In section III we present our results starting from these obtained for the model in which the values of the SO coupling constants are treated as the parameters and going to the realistic double quantum well heterostructure. The summary is contained in sec. IV.

II. THEORETICAL MODEL

A. Model of nanostructure

We consider the Datta and Das spin transistor architecture. Accordingly, the nanowire of width $W$ is located between two reflectionless leads acting as the spin polarizer and analyzer [see Fig. I(a)]. In order to ensure the high value of the on/off conductance ratio we assume 100% spin injection (detection) efficiency of the contacts, which as shown by recent experiments, 22–24 can be achieved using the QPC with the lateral Rashba SO interaction. Figure I(b) presents the cross-section of the layer heterostructure in the grown direction. We consider the Al$_{0.48}$In$_{0.52}$As/Ga$_{0.47}$In$_{0.53}$As double quantum well (width 50 nm) with a central barrier Al$_{0.3}$In$_{0.7}$As with width $w_b$ which determines the coupling between the conduction electron states in the quantum wells. The nanostructure contains two $n$-doped layers with donor concentrations $N_d = 4 \times 10^{18}$ cm$^{-3}$ and width 3 nm located on either side of the quantum well, 20 nm away from the well interface. In this nanodevice, the Rashba SO interaction can be tuned by the external gates with the lengths $L_g$ located below and above the quantum well, 50 nm away from the doping layers. By applying the suitably chosen voltages to these gates the spin transistor can be electrically switched between the on to off states as shown in Fig. I(e).

B. Hamiltonian with SO interaction

Here we briefly present the derivation of an effective Hamiltonian for conduction electrons with SO interaction. We start from the $8 \times 8$ Kane Hamiltonian for the layer heterostructure, which in the block form is given by 34:

$$H_{8\times8} = \begin{pmatrix} H_c & H_{cv} \\ H_{cv}^T & H_v \end{pmatrix},$$

where $H_c$ is the $2 \times 2$ diagonal matrix related to the conduction band ($\Gamma_6$ in the energy band profile - see Fig. III(c)) while $H_v$ is the $6 \times 6$ diagonal matrix corresponds to the valence bands ($\Gamma_8$, $\Gamma_7$ in the energy band...
FIG. 1. (a) Schematic of the spin transistor. Nanowire of width $W$ is located between two leads acting as the spin polarizer and analyzer. The spin dynamics in the conduction channel is controlled by the voltages applied to the gates $V_g$ and $V_a$.

(b) Cross section of $\text{Al}_{0.48}\text{In}_{0.52}\text{As}/\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$ double quantum well with a central barrier. (c) Band profile for the double quantum well with the central barrier. (d) Self-consistent potential energy profile and the corresponding wave functions $\varphi_1$ and $\varphi_2$. (e) $G(V_g)$ characteristics of the spin transistor with the marked on and off state.

Using the folding-down transformation, the $8 \times 8$ Hamiltonian (1) can be reduced into the $2 \times 2$ effective Hamiltonian for the conduction band

$$H(E)\psi_c = H_c + H_{cv}(E - H_v)^{-1}H_{vc}.$$  \hspace{1cm} (9)

Since $E_v$ and $\Delta_g$ are the largest energies in the system, we can expand the on- and off-diagonal elements of the Hamiltonian (9) in a series limiting to the first non-zero elements. This procedure leads to the Hamiltonian

$$H = \left[ \begin{array}{cc} -\frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} + \frac{\hbar^2}{2m_0} (k_x^2 + k_y^2) + V_{H}(z) + V_{\Gamma}(z) & 0 \\ 0 & \frac{\hbar}{2m_0} (k_y - ik_x) \end{array} \right]_{1 \times 2},$$  \hspace{1cm} (10)

where $V_{\Gamma}(z)$ is the self-consistent potential energy profile that can be expressed as

$$V_{\Gamma}(z) = h_0(z),$$  \hspace{1cm} (5)

$$V_{\Gamma}(z) = -h_0(z) - E_g,$$  \hspace{1cm} (6)

$$V_{\Gamma}(z) = -h_0(z) + E_g.$$  \hspace{1cm} (7)

where $h_0(z) = \delta_1h_{QW}(z) + \delta_2h_{b}(z)$ with $h_{QW}(z)$ being a dimensionless functions describing the potential energy profile of the quantum well (central barrier), $\delta_1(\delta_2)$ is the band-offset at the quantum well (central barrier) interface while $E_g$ and $\Delta_g$ are the energy gap and the split-off band gap, respectively.

The off-diagonal element $H_{cv}$ of the Hamiltonian (1) has the form

$$H_{cv} = \left( \begin{array}{cc} -\frac{\kappa}{\sqrt{2}} & \sqrt{2}k_z \\ 0 & \frac{\kappa}{\sqrt{2}} \end{array} \right),$$  \hspace{1cm} (8)

where $\kappa_{\pm} = \sqrt{\frac{E_g}{2E_g + \Delta_g}}$ is the conduction to valence band coupling with $|S\rangle, |X\rangle$ being the Bloch functions at the $\Gamma$ point.

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C. SO coupling constants

In this subsection, we briefly describe the procedure used to determine $\alpha(z)$ based on Eq. (13). The main part of this procedure contains the calculations of the self-consistent potential energy profile $V_{self}(z)$ which includes the band potential energy profile, the potential generated by the gates and doping and the Hartree potential resulting from the electron-electron interaction. In our calculations, we start from the single-electron Hamiltonian without the SO interaction and assume that the electron is confined in the $z$ direction while in the $x-y$ plane the system is infinite. This leads to the 1D Schrödinger equation in the form

$$\left(\frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} + \frac{\hbar^2 k^2}{2m^*} + V_{self}(z)\right) \varphi_n(z) = \varepsilon_n \varphi_n(z),$$

where $k^2 = k_x^2 + k_z^2$. The eigenproblem (17) is solved numerically by the diagonalization in the basis of infinite quantum well states $\varphi_n(z) = \sum_{j=1}^{N} c_j \sin(j\pi z/L_z)$, where $L_z$ is the total length of the heterostructure in the $z$ direction. The Hartree potential $V_H(z)$ [see Eq. (11)] is calculated from the Poisson equation

$$\frac{d^2}{dz^2} V_H(z) = -\frac{\varepsilon}{\epsilon_0 \epsilon_r} [n_e(z) + n_d(z)],$$

where $\varepsilon$ is the dielectric constant, $n_d(z)$ is the doping profile and $n_e(z)$ is the electron density, which is given by

$$n_e(z) = \frac{em^*}{\pi \hbar^2 k_B T} \sum_n \ln \left[ 1 + e^{(E_F - \varepsilon_n)/k_B T} \right]$$

where $k_B$ is the Boltzmann constant, $T$ is the temperature and $E_F$ is the Fermi energy. Equation (18) is solved by the relaxation method assuming the Dirichlet boundary conditions determined by the gate voltages. In calculations we always keep $V_g = 0$ as the reference potential. In the self-consistent procedure, equations (17) and (18) are solved iteratively until the convergence is reached. The self-consistent potential energy profile and the corresponding wave functions for two lowest states $\varphi_1$ and $\varphi_2$ are presented in Fig. 1(d). Then, the SO coupling $\alpha(z)$ is determined from the potential $V_{self}(z)$ by the use of Eq. (13). The present calculations have been performed for Al$_{0.48}$In$_{0.52}$As/Ga$_{0.47}$In$_{0.53}$As double quantum well with the following material parameters:

- $E_g = 0.8161$ eV, $\Delta_g = 0.3296$ eV, $\delta_b = 0.52$ eV, $\delta_f = 0.1637$ eV, $\delta_8 = 0.1935$ eV, $\delta_{56} = 0.21$ eV, $\delta_{17} = 0.1343$ eV, $\delta_{58} = 0.152$ eV, $m^* = 0.043$ and $E_F = 2m_0 P^2/\hbar^2 = 25.3$ eV. The dielectric constant $\epsilon_r = 14.013$ is assumed to be constant in the entire heterostructure.

D. Effective 2D Hamiltonian and conductance calculations

Now, we derive an effective 2D Hamiltonian in the two subband model starting from its 3D version given by Eq. (10). For this purpose we define the four element basis $\{ |\varphi_1, \uparrow\rangle, |\varphi_1, \downarrow\rangle, |\varphi_2, \uparrow\rangle, |\varphi_2, \downarrow\rangle \}$ which consists of the spin-degenerate ground and first excited eigenstate of the Hamiltonian (17) without SO interaction. The projection of (10) onto this basis leads to the $4 \times 4$ Hamiltonian given by

$$\mathcal{H}_{2D} = \begin{pmatrix}
\frac{\hbar^2 k_x^2}{2m^*} + \varepsilon_1 & \alpha_{11}(k_y + ik_z) & 0 & \alpha_{12}(k_y + ik_z) \\
\alpha_{11}(k_y - ik_z) & \frac{\hbar^2 k_z^2}{2m^*} + \varepsilon_1 & \alpha_{12}(k_y - ik_z) & 0 \\
0 & \alpha_{12}(k_y + ik_z) & \frac{\hbar^2 k_x^2}{2m^*} + \varepsilon_1 & \alpha_{22}(k_y + ik_z) \\
0 & \alpha_{12}(k_y - ik_z) & \alpha_{22}(k_y - ik_z) & \frac{\hbar^2 k_z^2}{2m^*} + \varepsilon_2
\end{pmatrix}$$

where $\alpha_{nm} = \langle \varphi_n | \alpha(z) | \varphi_m \rangle$ with $n, m = 1, 2$.

The calculations of the conductance have been performed within the scattering matrix method using the Kwant package. For this purpose we have transformed the Hamiltonian (20) into the discretized form on the grid $(x_\mu, y_\nu) = \mu dx, \nu dx$ ($\mu, \nu = 1, 2, \ldots$) where $dx$ is the lattice constant. We introduce the discrete representation of the electron state in the $4 \times 4$ space as follows: $|\Psi(x_\mu, y_\nu)\rangle = (|\psi_1^+ (x_\mu, y_\nu), |\psi_1^- (x_\mu, y_\nu), |\psi_2^+ (x_\mu, y_\nu), |\psi_2^- (x_\mu, y_\nu)\rangle)^T$. Introducing a set $\tau$ of Pauli-like matrices in the orbital space, the Hamiltonian (20) takes on the dis-
cretized form
\[ \mathcal{H}_{2D} = \sum_{\mu\nu} \left[ (4t + \varepsilon_{+}) \mathbf{1} \otimes \mathbf{1} - \varepsilon_{-} \tau_{z} \otimes \mathbf{1} \right] |\Psi_{\mu,\nu}\rangle \langle \Psi_{\mu,\nu}| \\
+ \sum_{\mu\nu} \left\{ t(1 \otimes 1 + it_{SO} \left[ \alpha_{11} \frac{1}{2} (1 - \tau_{z}) \otimes \sigma_{y} \right. \right.
\left. \left. + \alpha_{12} \frac{1}{2} (1 + \tau_{z}) \otimes \sigma_{y} \right) + H.c. \right\} + \sum_{\mu\nu} \left\{ t(1 \otimes 1 + it_{SO} \left[ \alpha_{11} \frac{1}{2} (1 - \tau_{z}) \otimes \sigma_{x} \right. \right.
\left. \left. + \alpha_{12} \frac{1}{2} (1 + \tau_{z}) \otimes \sigma_{x} \right) + H.c. \right\}, \tag{21} \]

where \( t = \hbar^{2}/(2mdx^{2}) \), \( t_{SO} = 1/(2dx) \) and \( \mathbf{1} \) is the \( 2 \times 2 \) unity matrix.

Let us assume that the electron with spin up in the first subband is injected from the source (polarizer) into the conduction channel. The electron can be transmitted via the conduction channel to the analyzer in one of the four possible processes: (i) intra-subband transmission with spin conservation \( (T_{11}^{\uparrow \uparrow}) \), (ii) intra-subband transmission with spin-flip \( (T_{11}^{\uparrow \downarrow}) \), (iii) inter-subband transmission with spin conservation \( (T_{12}^{\uparrow \uparrow}) \) and (iv) inter-subband transmission with spin flip \( (T_{12}^{\uparrow \downarrow}) \), where \( T_{nm}^{\sigma\sigma'} \) with \( \sigma, \sigma' = \uparrow, \downarrow \) and \( n, m = 1, 2 \) denotes the probabilities of the transmission processes (i) - (iv). Similar scattering processes can be introduced for the spin-up electrons injected from the second subband. Their probabilities are denoted by \( T_{22}^{\uparrow \uparrow}, T_{22}^{\uparrow \downarrow}, T_{21}^{\uparrow \uparrow}, T_{21}^{\uparrow \downarrow} \).

Having determined the transmission coefficients \( T_{nm}^{\sigma\sigma'} \), we calculate the conductance in the ballistic regime using the Landauer formula
\[ G_{nm}^{\sigma\sigma'} = \frac{e^{2}}{\hbar} \int T_{nm}^{\sigma\sigma'}(E) \left( \frac{\partial f_{FD}(E, E_{F})}{\partial E} \right) dE, \tag{22} \]
where \( \sigma, \sigma' \) are the spin indices and \( f_{FD}(E, E_{F}) = \frac{1}{[1 + \exp(E - E_{F})/k_{B}T]} \) is the Fermi-Dirac distribution function, where \( T \) is the temperature and \( E_{F} \) is the Fermi energy.

For the assumed 100% spin injection (detection) efficiency of the contacts, the total conductance via the device is given by
\[ G = \sum_{n, m=1}^{2} G_{nm}^{\uparrow \uparrow}. \tag{23} \]
The conductance calculations presented in the paper have been performed for \( dx = 2 \text{ nm} \) and \( T = 4.2 \text{ K} \).

III. RESULTS

In this section we study the conductance through the spin transistor including the intra- and inter-subband SO interaction. We start from the model, in which the SO coupling constants are treated as the parameters (subsection A) and show how the inter-subband-induced SO coupling affects the spin transistor operation. Then, in subsection B, we introduce the realistic model with the Al0.48In0.52As/Ga0.47In0.53As double quantum well, for which the SO coupling constants are determined by the Schrödinger-Poisson approach presented in subsection C.

A. Parametrized model

We consider the spin transistor with the length \( L = 800 \text{ nm} \) and the gate attached to the conduction channel in the middle of the nanostructure. The length of the gate \( L_{g} = 400 \text{ nm} \) (see Fig. I). The energy difference between the two subbands is taken to be \( \Delta\varepsilon = \varepsilon_{2} - \varepsilon_{1} = 1 \text{ meV} \) [Eq. (20)]. We assume the channel width \( W = 40 \text{ nm} \) which guarantees that the energy separation between the two lowest energy states related to the confinement in the lateral \( y \) direction \( \Delta\varepsilon_{y} \approx \hbar^{2} \pi^{2}/2m^{*}W^{2} = 4.2 \text{ meV} \) is greater than \( \Delta\varepsilon \). All results presented in this subsection have been obtained for the Fermi energy \( E_{F} = 4 \text{ meV} \), which ensures that only the lowest energy state in the transverse motion \( (y \text{ direction}) \) is occupied and the two subbands in the grown \( z \) direction participate in the transport. The SO coupling constants, experimentally controlled by the gate voltage, are treated as the parameters of the calculations.

Let us start our study from the case in which the intra-subband SO coupling constants, in the both subbands are equal \( \alpha_{11} = \alpha_{22} = \alpha \). Figure 2 presents the conductance as a function of \( \alpha \) for different inter-subband SO coupling constant \( \alpha_{12} \). We assume that \( \alpha_{12} \) takes on the negative values which is consistent with the results for the realistic structure (see subsection B). As we have checked, the change of sign \( \alpha_{12} \) does not change the conductance in any way – the conductance depends only on the absolute value of \( \alpha_{12} \). For the inter-subband SO coupling constant \( \alpha_{12} = 0 \) the spin dynamics in the two subbands, via which the electrons are transmitted, is independent. The spin of electron flowing in the vicinity of the gate rotates due to the SO interaction. Since the intra-subband SO coupling are assumed to be equal, the electron spin in each of the subbands precesses with the same precession length \( \lambda_{SO} = 2\pi/\Delta\kappa \), where \( \Delta\kappa = k_{F} - k_{F} = 2m^{*}\alpha/\hbar^{2} \). In this case, the slight difference in the transport conditions through the both subbands can result from the energy difference \( \Delta\varepsilon \), however it is too small to affect the spin transistor operation. Hence, if we assume the ideal spin polarizer (analyzer), which transmits only electrons with well defined spin, the conductance oscillates as a function of \( \alpha \) according to the formula
\[ G = 2G_{0}\cos^{2} \left( \frac{\Delta\kappa L_{g}}{2} \right) = 2G_{0}\cos^{2} \left( \frac{m^{*}\alpha L_{g}}{\hbar^{2}} \right), \tag{24} \]
where \( G_{0} = e^{2}/\hbar \) and the factor 2 is related to the fact
that the electrons are transmitted via the two subbands. These conductance oscillations as a function of the intra-subband SO coupling constant \( \alpha \) are presented in Fig. 2 (black line, \( \alpha_{12} = 0 \)). Based on Eq. (24) one can conclude that the conductance reaches maximum for \( \Delta k L_g = 2N\pi \), which corresponds to the process, in which the spin of the electron flowing through the conduction channel precesses the integer number of times. On the other hand, the conductance minimum is reached for \( \Delta k L_g = (2N + 1)\pi \), which corresponds to the half-integer rotation number of the electron spin. The former case is depicted in the inset of Fig. 2 in which we present the spin density distributions \( s_z^{(1,2)} \) for the first (1st) and second (2nd) subband for \( \alpha = 14 \text{ meVnm} \) and \( \alpha_{12} = 0 \).

The regular oscillations of \( G(\alpha) \) are modified if we introduce the inter-subband SO coupling into the system, i.e. \( \alpha_{12} \neq 0 \). As presented in Fig. 2 for \( \alpha_{12} = -10 \text{ meVnm} \) the change of the conductance becomes significant for large values of \( \alpha \). The black and red line come together for small \( \alpha \) and diverge for \( \alpha > 10 \text{ meVnm} \). For \( \alpha = 14 \text{ meVnm} \), marked by the vertical dashed line, the inter-subband SO interaction leads to the slight reduction of the conductance. The further change of the inter-subbands SO coupling constant up to \( \alpha_{12} = -18 \text{ meVnm} \) leads to the inversion of the oscillations, namely the conductance reaches the minimum for \( \alpha \) for which it is maximal in the case of \( \alpha_{12} = 0 \). This inversion is clearly visible in Fig. 3 which presents the conductance as a function of the intra- and inter-subband SO coupling constants \( G(\alpha, \alpha_{12}) \). The complete inversion is observed for \( \alpha_{12} = -18 \text{ meVnm} \) (white dashed line), for which also the period of the \( G(\alpha) \) oscillations slightly increases. Interestingly, as presented in Fig. 3(b) even for \( \alpha = 0 \) corresponding to the symmetric heterostructure, the conductance oscillates as a function of \( \alpha_{12} \). The transmission probabilities shown in Fig. 3(c) indicate that this behavior is directly related to the increase of the inter-subbands spin-flip transmission probability. All these results suggest the possible application of the inter-subband SO interaction in the spin transistor design, although the experimental control of \( \alpha_{12} \) still remains an open issue.

The conductance behavior [Figs. 2 and 3] result from the spin dynamics, which in the presence of the inter-subband SO interaction becomes much more complicated. Similarly, as for \( \alpha_{12} = 0 \), the spin dynamics is determined by the differences of \( k_F \) Fermi wave vector between the subbands participating in the transport for the given Fermi energy. These differences can be determined from the eigenenergies of Hamiltonian (20), which are given by

\[
E_{ksp} = E_0 + \frac{\hbar^2 k^2}{2m^*} + \varepsilon_+ + s\alpha + k + \rho \sqrt{(\alpha_{12} k)^2 + (\varepsilon_- + s\alpha - k)^2},
\]

where

\[
\varepsilon_\pm = \frac{1}{2}(\varepsilon_1 \pm \varepsilon_2), \quad \alpha_\pm = \frac{1}{2}(\alpha_1 \pm \alpha_2),
\]

\( E_0 \) is the energy of the lowest state related to the confinement in the lateral \( y \) direction while \( s = \pm 1 \) and \( \rho = \pm 1 \) correspond to the spin state and the subband, respectively.

Notice, that the electron initially injected into the channel within spin up state oscillates between the subbands changing its spin. The spin dynamics is the combination of the precession with different precession lengths which, in contrast to the case with \( \alpha_{12} = 0 \), depend on the Fermi energy. The simplest case for which this problem can be solved analytically is the symmetric structure with zero intra-subband SO coupling (\( \alpha = 0 \)), presented in Fig. 3(b). Then, the spin precession length is given by

\[
\lambda_{SO} = \frac{2\pi}{\Delta k} = \frac{2\pi}{k_2 - k_1},
\]

where
In Fig. 4 we present the $z$ component $s_z^{1(2)}$ of the spin density distribution for the both subbands and $\alpha_{12} = -18$ meVnm corresponding to the conductance minimum in Fig. 3(b). The lower panels in Fig. 3 depict the partial spin density distributions: (I) $s_z^{11}$ and (II) $s_z^{12}$ correspond to the spin density distribution in the first and second subband, respectively, if the electron with spin up is injected into the first subband, while $s_z^{21}$ (III) and $s_z^{22}$ (IV) correspond to the spin density distribution in the first and second subband, if the electron with spin up is injected into the second subband. These partial spin density distributions give us information not only about the spin dynamics in the considered subband but also about the spin behavior due to the inter-subband transitions.

For the both subbands (Fig. 4) the electrons initially injected with spin up reverse their spin when flowing through the nanodevice [cf. $s_z^1$ and $s_z^2$]. The spin-down electrons reaching the output are backscattered from the ideal spin-up polarized contact (analyzer), which leads to the decrease of the conductance presented in Fig. 3(b). Since the intra-subband SO coupling constant $\alpha = 0$ the spin of the electron flowing through the subband, in which it was injected, does not precess [cf. Figs. 3 (I) and (IV)]. Nevertheless, as presented in Fig. 3 (II) and (III) the electron spin is inverted in the inter-subband transitions, the probability of which reaches maximum for the chosen $\alpha_{12}$. In this case, the spin precession length is given by Eq. (27).

The spin dynamics near the gate becomes more complicated for the nonzero intra-subband SO coupling ($\alpha \neq 0$). In this case the spin degeneracy of the subbands is lifted. Thus, beside the reversal of spin related to the inter-subband transition, we expect the intra-subband spin

\begin{align*}
k_1 &= \frac{\sqrt{2m^*E_F}}{\hbar} \sqrt{1 - \frac{\varepsilon_+}{E_F} + \frac{\alpha^2_{12}m^*}{\hbar^2 E_F} \left( 1 + \frac{\sqrt{1 + 2h^2(E_F - \varepsilon_-) + \frac{\hbar^4\varepsilon_-^2}{\alpha^4_{12}m^* + \hbar^4\varepsilon_-^2}}}{\alpha^2_{12}m^* + \hbar^4\varepsilon_-^2} \right) } , \quad (28) \\
k_2 &= \frac{\sqrt{2m^*E_F}}{\hbar} \sqrt{1 - \frac{\varepsilon_+}{E_F} + \frac{\alpha^2_{12}m^*}{\hbar^2 E_F} \left( 1 - \frac{\sqrt{1 + 2h^2(E_F - \varepsilon_-) + \frac{\hbar^4\varepsilon_-^2}{\alpha^4_{12}m^* + \hbar^4\varepsilon_-^2}}}{\alpha^2_{12}m^* + \hbar^4\varepsilon_-^2} \right) } . \quad (29)
\end{align*}
precession. In Fig. 5 we present the spin density distributions for $\alpha = 14$ meVnm (marked by the vertical dashed line in Fig. 2) and two chosen values of the inter-subband SO coupling constants (a) $\alpha_{12} = -10$ meVnm and (b) $\alpha_{12} = -18$ meVnm. As shown in Fig. 5 for $\alpha_{12} = -10$ meVnm the spin dynamics in the nanostructure differs only slightly from the case without the inter-subband SO interaction (compare with the inset of Fig. 2). The electron spin performances one full rotation and leaves the nanodevice with almost the same spin as on the input. In contrast to the case with $\alpha_{12} = 0$, we observe the inter-subband transition in which the electron conserves its spin. The spin dynamics drastically changes if we increase the inter-subband SO coupling. For $\alpha_{12} = -18$ meVnm [Fig. 5(b)] the electrons initially injected with spin up reverse their spin on the output leading to the decrease of the conductance. Note that in contrast to the spin dynamics for $\alpha = 0$, for which the spin flip is related to the inter-subband transition, in the case of $\alpha \neq 0$ the electron conserves the spin in this type of transitions. Due to the intra-subband SO interaction the spin precession takes place mainly in the subband into which the electron is injected. However this precession is strongly affected by the inter-subband SO interaction, which significantly changes the precession length.

$$\beta_n = \beta^{3D} \langle \varphi_n | k_z^2 | \varphi_n \rangle,$$

(30) where $\beta^{3D}$ is the Dresselhaus SO coupling for the bulk taken on as $\beta^{3D} = 0.0237$ meVnm$^3$. Figure 7 shows that for the considered wide quantum well, the Dresselhaus SO coupling constants $\beta_{1(2)}$ are two orders of magnitude smaller than the Rashba constants [Fig. 7(d)]. Therefore, the Dresselhaus SO interaction is neglected in the conductance calculations presented in the rest of the paper.

Figure 7(c) shows that the inter-subband SO coupling constant is an even function of the gate voltage and exhibits the "resonant behavior" around $V_g = 0$ corresponding to the symmetric geometry of the heterostructure. Simultaneously, at the resonant voltage $V_g = 0$, the intra-subband SO coupling constants $\alpha_{11}$ and $\alpha_{22}$ change the sign. Similar "resonant behavior" was recently reported by Calsaverini et. al. for InSb/Al$_{0.12}$In$_{0.88}$Sb double quantum well. The authors argued that this feature results from the dominant role of the Hartree potential and the overlap between the wavefunctions of the ground and the first excited state in the quantum well, which for $V_g = 0$ becomes maximal. Notice that the conductance channel, in which the SO coupling constants rapidly change around $V_g = 0$ is preferred for the application in the spin transistor architecture in which the switching between the on and off states should be realized in the gate voltage range as narrow as possible [see Fig. 7(c)]. We have performed the calculations of Rashba constants for different electron densities (Fig. 7) taking care that only the two lowest-energy states in the quantum well were occupied. As shown in Fig. 7 the increasing electron density $n_e$ leads to the increase of the slope $\alpha_{11(22)}(V_g)$ curves around $V_g = 0$ making the heterostructure more convenient for the spin transistor application. Simultaneously, the inter-subband SO coupling
\( \alpha_{12} \) at \( V_g = 0 \) decreases which, as we will show later, also affects the conductance at this gate voltage.

Having the SO coupling constants determined from the Schrödinger-Poisson approach we calculate the conductance using of the scattering matrix method. For this purpose we consider the spin transistor with length \( L = 3 \mu m \), width \( W = 40 \) nm and the gate located in the middle of the conduction channel. The length of the gate \( L_g = 2 \mu m \) is assumed to be comparable to that used in recent experiment. Figure \( 8(a) \) depicts the conductance as a function of gate voltage for different electron densities. The conductance \( G(V_g) \) exhibits the pronounced peak around \( V_g = 0 \) related to the low resistance state of the spin transistor (on state). The change of the gate voltage in the narrow range around \( V_g = 0 \) switches the transistor into the low conductance state with the high resistance (off state). Notice that the on/off conductance ratio strongly depends on the electron density and is larger for high \( n_e \). The dependence \( G(V_g) \) is determined by the spin dynamics in the conduction channel, which depends on the strength of the Rashba SO interaction. At \( V_g = 0 \) related to the symmetric geometry of the heterostructure, the intra-subband SO coupling constants \( \alpha_{11} = \alpha_{22} = 0 \) [see Fig. \( 7(a)(b) \)]. Then, in the absence of the inter-subband SO interaction, the spin of the electron injected from the polarizer does not precess and the electron leaves the conduction channel with the same spin matching the polarization of the left contact (analyzer). The both subbands transmit the electrons giving rise to the conductance \( G = 2e^2/h \). However, as shown in Fig. \( 7(a) \) and (b) the slight deviation of the gate voltage from \( V_g = 0 \) causes the rapid change of the intra-subband SO coupling constants. In particular, if the strength of this SO interaction is sufficient to inverse the spin of the electron flowing through the nanostructure the electron is reflected from the analyzer, which results in the zero conductance. As shown in Fig. \( 7(a) \) the large changes of the conductance around \( V_g = 0 \) are strictly related to the abrupt change of the SO coupling constants presented in Fig. \( 7 \). Outside the close vicinity of \( V_g = 0 \) the conductance is almost constant, which results from the nearly constant values of the SO coupling in this range (see Fig. \( 7 \)).

The model of spin dynamics presented above is correct in the absence of the inter-subband-induced SO interac-

\( \alpha_{12} \) and \( \alpha_{22} \) and inter-subband (c) \( \alpha_{12} \) SO coupling constants as a function of gate voltage \( V_g \) for different electron densities \( n_e \). (d) Dresselhaus SO coupling constants as a function of gate voltage \( V_g \) for \( n_e = 10 \times 10^{11} \) cm\(^{-2} \).
FIG. 9. Transmission probabilities $T$ as a function of gate voltage $V_g$ for the electron density (a) $n_e = 4 \times 10^{11}$ cm$^{-2}$ and (b) $n_e = 10 \times 10^{11}$ cm$^{-2}$.

FIG. 10. Intra-subband (a) $\alpha_{11}$ and (b) $\alpha_{22}$ and inter-subband (c) $\alpha_{12}$ SO coupling constants as a function of gate voltage $V_g$ for different barrier widths $w_b$. (d) Energy separation between the subbands $\Delta \epsilon = \epsilon_2 - \epsilon_1$ at $V_g = 0$ as a function of barrier width $w_b$. Results for $n_e = 10 \times 10^{11}$ cm$^{-2}$.

FIG. 11. (a) Conductance $G$ as a function of gate voltage $V_g$ for different barrier widths $w_b$. (b) Inter-subband transmission with spin conservation $T_{\uparrow\uparrow}^{12}$ and (c) inter-subband transmission with spin flip $T_{\uparrow\downarrow}^{12}$ as a function of gate voltage $V_g$. 

For the low electron density $n_e = 4 \times 10^{11}$ cm$^{-2}$ the inter-subband SO interaction is absent both for electrons injected from the first and the second subband. The decrease of the conductance for $V_g \neq 0$ corresponds to the increase of the intra-subband transmission with spin flip. For the high electron density $n_e = 10 \times 10^{11}$ cm$^{-2}$ the probability of the inter-subband transmissions is nonzero.
around $V_g = 0$. Notice that at $V_g = 0$ the inter-subband transmission always accompanies the spin flip while the probability of the inter-subband transmission with spin conservation $T_{12}^{↑↑} = T_{21}^{↑↑} = 0$. It is worth mentioning that the transmission probabilities for positive and negative gate voltages are not equivalent leading to the non-symmetric dependence $G(V_g)$ presented in Fig. 5. This asymmetry emerges for high gate voltages for which the inter-subband SO interaction is weak. Hence, it results from the asymmetry of the intra-subband SO coupling constants for the ground and first excited state which is analogous to that observed in Fig. 6.

As shown above the conductance in the vicinity of $V_g = 0$ is mainly determined by the inter-subband transitions which emerge in the system as a result of the inter-subband SO interaction. This leads to the question how the width of the central barrier $w_b$, which directly determines the coupling between the quantum wells, affects the conductance in the considered gate voltage range. In Fig. 10(a)-(c) we present the intra- and inter-subband SO couplings as a function of the gate voltage calculated for different barrier widths. Figure 10(a) shows that the resonant behavior of $\alpha_{12}$ is more pronounced for the wide central barrier, while the width of the barrier almost does not change the value of $\alpha_{12}$ at $V_g = 0$. In addition, the slopes $d\alpha_{11}/dV_g$ and $d\alpha_{22}/dV_g$ at $V_g = 0$ increase with the increasing $w_b$, making the system more suitable for the spin transistor application. However, as presented in Fig. 10(a), the conductance at $V_g = 0$ is strongly reduced for the wide barrier giving rise to the low on/off conductance ratio. This effect results from the inter-subband transmissions the probabilities of which are presented in Figs. 11(b) and (c). Both these figures clearly indicate that the reduction of $G(0)$ is due to the inter-subband transmission with spin-flip. However, we note that $\alpha_{12}$ at $V_g = 0$ is nearly constant and is almost independent on on the barrier width [Fig. 10(c)]. Therefore, we conclude that the increase of $T_{12}^{↑↓}$ is mainly caused by the reduction of $\Delta \varepsilon$ [cf. Fig. 10(d)], which decreases with the increasing barrier width - the reduction of the coupling between quantum wells considerably weakens the repulsion of the states.

IV. SUMMARY

The inter-subband-induced SO interaction in the quantum well with the double occupancy has attracted the growing interest because it can give rise to interesting physical effects, e.g. unusual Zitterbewegung. This specific SO interaction is nonzero even in the symmetric heterostructure, as it arises from the coupling between states with opposite parity. The strength of this coupling is comparable to the ordinary Rashba intra-subband SO coupling. In the present paper we have analyzed the influence of the inter-subband SO interaction on the spin transistor operation. For this purpose, we have calculated the electron transport in the spin transistor within the two-subband model including both the intra- and inter-subband SO interaction. We have started from the model in which the SO coupling constants are treated as the parameters. In the absence of the inter-subband SO interaction and with equal intra-subband SO coupling constants we have obtained the regular conductance oscillations, similar to those predicted for the quantum well with the single occupancy. We have shown that these oscillations are strongly affected by the inter-subband SO interaction leading to its irregular and damped form. For large $\alpha_{12}$ we have found the inversion of the oscillations, i.e., the conductance maxima and minima interchange. Interestingly, we have demonstrated that even for the zero intra-subband SO coupling related to the symmetric geometry, the conductance oscillates as a function of the inter-subband SO coupling. This effect has been explained as resulting from the inter-subband transitions with spin flip. Finally we have also performed calculations with the asymmetry of the intra-subband SO coupling constants. As we found the inter-subband SO interaction lifts the symmetry of the conductance with respect to the subbands interchange.

In the second part of the paper, we have studied the conductance within the realistic spin transistor model with the conduction channel based on the Al$_{0.48}$In$_{0.52}$As/Ga$_{0.47}$In$_{0.53}$As double quantum well. For the considered nanostructure, by performing a detailed self-consistent calculations in which we solve both Poissons and Schrödinger equation iteratively, we have determined the strengths of the SO coupling contacts $\alpha_{11}$, $\alpha_{22}$ and $\alpha_{12}$. The values of these coupling constants contain contributions arising from the potential-well and barrier offsets, the Hartree potential, the external gate potential and the modulation doping potential. We have obtained the resonant behavior of $\alpha_{12}$ versus the gate voltage. Furthermore, the intra-subband SO coupling rapidly changes its sign and magnitude at $V_g = 0$. As we have stated in the paper such a rapid change of the SO coupling constants in the narrow voltage range is favorable for the spin-FET application in which the on/off conductance switching should be realized in the possibly narrow gate voltage. Our calculations for different electron densities have shown that this effect can be strengthened for the high electron concentration in the quantum well. However, for the high electron density the inter-subband SO interaction becomes dominant. The suppression of the conductance at $V_g = 0$ which results from the inter-subband transition with spin flip is the strong evidence of this interaction. This effect leads to the reduction of the on/off conductance ratio. Similar effect has been observed for the wide central barrier, for which the increase of the inter-subband transmissions is mainly due to the decrease of the energy separation between both the subbands with almost constant $\alpha_{12}$.

In summary, our studies of the inter-subband SO interaction on the spin transistor operation show that this SO coupling leads to the reduction of the on/off conductance ratio and thus decreases the efficiency of the spin
transistor.

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* Electronic address: pawel.wojcik@fis.agh.edu.pl

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