General condition for realizing a collinear spin-orbit effective magnetic field in two-dimensional electron systems and its application to zinc-blende and wurtzite quantum wells

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In this paper, we have studied two-dimensional (2D) electron systems described by the effective Hamiltonians containing spin-orbit coupling (SOC) terms up to an arbitrary odd order in wave vector \mathbf{k} . The general condition for realizing a SOC-induced effective magnetic field (SOF) in such systems, formulated only in terms of the SOC parameters, is derived. When this condition is satisfied, the projection of the electron spin on the direction of the collinear SOF is a conserved quantity. The complete set of the \mathbf{k} -linear and \mathbf{k} -cubic Dresselhaus SOC contributions to the effective 2D Hamiltonian of an arbitrarily oriented zinc-blende quantum well is computed by a proper averaging of the corresponding tight-binding bulk SOC Hamiltonian. We investigate possibilities for realization of the collinear SOF in zinc-blende quantum wells of different orientation and obtain some interesting findings, which supplement the results of earlier works. Application of the developed formalism to wurtzite semiconductor 2D systems shows that the collinear SOF can be also realized in a wide class of such quantum wells.

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I. INTRODUCTION

The achievement of long enough spin lifetimes is essential for fabrication of spintronic devices [1,2]. In the last 15 years, several two-dimensional electron systems (2DES) with appropriate properties were found. In 2003 Schliemann et al. [3] proposed a nonballistic spin-field-effect transistor based on a [001] zinc-blende (ZB) quantum well (QW) with the Rashba and Dresselhaus spin-orbit coupling (SOC) terms of equal strengths. Later, Bernevig et al. [4] connected unique features of this system with a type of SU(2) spin rotation symmetry and found that one is also realized in symmetric [110] ZB QWs. In addition, in that paper the persistent spin helix, which is a special spin precession pattern with the precession angle depending only on the net displacement in specific directions (\pm [110] for [001] QWs with equal SOC strengths and $[1\overline{1}0]$ for symmetric [110] QWs), was predicted. Presently, different aspects of the persistent spin helices were studied in many theoretical [5–15] and experimental [16–23] works (the key developments in both theory and experiment are summarized in Ref. [24]).

Formation of the collinear SOC-induced effective magnetic field (SOF) is another feature of 2DES with additional spin symmetry. In general, the direction of the SOF field depends on the wave vector $\mathbf{k} = \{k_x, k_y\}$ of the electron. Hence, spins of the carriers propagating along different directions in the QW plane precess in different ways. Nevertheless, in the symmetric cases the SOF is collinear to a peculiar direction, which is determined only by the SOC parameters, and the projection of the electron spin on this direction is a conserved quantity.

Kammermeier *et al.* [25] considered the model Hamiltonian for the lowest conduction subband in direct bandgap ZB QWs obtained after averaging of the bulk Dresselhaus Hamiltonian [26] along an arbitrary crystallographic direction [hkl], which coincides with the growth direction of the corresponding OW. The authors found that if the k-linear SOC terms are taken into account the collinear SOF can be realized only in QWs with at least two equal in modulus growth direction Miller indices. In our previous works [27,28], slightly subsequent to work [25], we proposed a similar condition for realization of the collinear SOF in 2DES described by the Hamiltonian with the generalized k-linear SOC contributions. This condition is formulated only in terms of the SOC parameters of the effective 2D Hamiltonian and is applicable not only for ZB QWs, but also for the other 2DES that are described by the Hamiltonian of such a type (for instance, wurtzite 2DES and SiGe QWs). In this paper, we generalize this result considering the effective 2D Hamiltonian containing SOC terms up to an arbitrary odd in **k** order and derive the general condition for realizing a collinear SOF in the presence of these terms.

In general, nonlinear in k SOC terms constitute an obstacle for the realization of SU(2) symmetry. Despite that, a conserved spin quantity and a collinear SOF exist in the presence of k-cubic or even SOC contributions of a higher order in k in some exceptional cases. In the supplemental material of Ref. [25] the influence of k-cubic Dresselhaus SOC terms on the collinearity of the effective SOF in ZB QWs was discussed. Under these circumstances, it was found that the collinear SOF can be realized in the presence of the Dresselhaus cubic terms only in symmetric [110] QWs or asymmetric [111] QWs with the Rashba and Dresselhaus k-linear SOC contributions compensating each other. In these calculations, however, k-cubic Rashba SOC terms were neglected. Moreover, in Ref. [29] it was shown that the conventional 2D spin Hamiltonians for [001], [110], and [111] ZB QWs derived in Ref. [26] should be supplemented by additional k-cubic Dresselhaus SOC terms to account for all SOC effects. In this paper, we compute the complete set of the linear and cubic Dresselhaus SOC contributions to the effective 2D spin Hamiltonian of ZB QWs by averaging along the growth direction the bulk Dresselhaus Hamiltonian of fifth order in **k** within the lowest conduction subband. We also employ the known expressions for **k**-cubic Rashba SOC terms in ZB QWs of certain orientations [29] to reexamine possibilities for realization of the collinear SOF in the presence of the cubic SOC terms in such QWs.

This paper is organized as follows. In Sec. II, we introduce the effective 2D Hamiltonian containing SOC terms up to 2n + 1 in wave vector **k** order and derive the general condition for realizing a collinear SOF in 2DES. Therein, we discuss in detail two particular cases of this condition corresponding to the generalized k-linear (n = 0) and k-cubic (n = 1) SOC Hamiltonians. In Sec. III, we compute the complete set of the k-linear and k-cubic Dresselhaus SOC contributions to the effective 2D spin Hamiltonian of an arbitrarily oriented ZB QW by averaging along the growth direction the relevant bulk Dresselhaus Hamiltonian of fifth order in k within the lowest conduction subband. In Sec. IV, we investigate possibilities for realization of the collinear SOF in [001]-, [110]-, [111]-, [113]-, and [013]grown ZB QWs. Results of application of the developed formalism to wurtzite 2DES are presented in Sec. V. Finally, the paper is summarized in Sec. VI.

II. THE GENERAL CONDITION FOR REALIZING A COLLINEAR SOF

In general, the existence of an extra symmetry connected with the spin degree of freedom leads to conservation of the spin density projection on a specific direction that is characterized by a unit vector $\mathbf{n} = \{n_x, n_y, n_z\}$ [3,24]. In the framework of the single-particle approximation it is expressed as

$$[\hat{H}, \hat{\Sigma}] = \hat{0}. \tag{1}$$

Here, \hat{H} is the Hamiltonian containing SOC terms and

$$\hat{\Sigma} = \left(\mathbf{n} \cdot \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}\right) = \frac{\hbar}{2}(n_x\hat{\sigma}_x + n_y\hat{\sigma}_y + n_z\hat{\sigma}_z) \qquad (2)$$

is the operator of the spin projection on the direction **n**, where $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ are the Pauli matrices. For 2DES with the additional spin symmetry vector **n** also determines the direction of the collinear SOF [24,25,27]. Hence, the condition (1) can be regarded as a starting point for identification of 2DES with the collinear SOF.

Different types of 2DES with SOC are described by effective Hamiltonians, where the structure is defined, in fact, by only two symmetry restrictions: presence of the time reversal symmetry and absence of the space-inversion symmetry. Therefore, the SOC part of the effective Hamiltonian is constructed as a sum of products of the Pauli matrices and odd combinations of the wave vector components [30]. In any particular case, the functional form of the SOC part can be purely determined from symmetry considerations by means of either the invariant expansion of the Hamiltonian method [31] or the double group tight-binding method [29]. In order to achieve our goals formulated above, we consider the following effective Hamiltonian:

$$\hat{H} = \mu \left(\hat{k}_x^2 + \hat{k}_y^2 \right) \hat{\sigma}_0 + \sum_{j=0}^n \hat{H}_{\text{SO}}^{(2j+1)},$$
(3)

where

$$\hat{H}_{\rm SO}^{(2j+1)} = \sum_{t=0}^{2j+1} \sum_{s=1}^{3} \gamma_{s,t,\ 2j+1-t} \,\hat{\sigma}_s \hat{k}_x^t \hat{k}_y^{2j+1-t}.$$
 (4)

Here, we use Cartesian coordinates with the *z* axis perpendicular to the plane of two-dimensional electron gas (2DEG), $\hat{\sigma}_0$ is 2 × 2 unit matrix, $\hat{\mathbf{k}} = \{\hat{k}_x, \hat{k}_y\} = -i\nabla$, $\mu \equiv \hbar^2/2m$, where *m* is the effective electron mass, and real parameters γ_{abc} define the asymmetry induced SOC. We include in the spin-independent part of the Hamiltonian (3) only the usual quadratic in $\hat{\mathbf{k}}$ kinetic energy of the electron. The even terms of higher orders (for instance, quartic) that are still consistent with the time-reversal symmetry will not be considered in the following because the results presented below do not depend on the presence of such terms.

As a rule, only the linear (j = 0) and cubic (j = 1) in wave vector SOC terms are taken into account in the sum in the Hamiltonian (3). In this case, it is reduced to

$$\hat{H} = \mu \left(\hat{k}_x^2 + \hat{k}_y^2 \right) \hat{\sigma}_0 + \hat{H}_{\rm SO}^{(1)} + \hat{H}_{\rm SO}^{(3)}, \tag{5}$$

where

$$\hat{H}_{SO}^{(1)} = (\gamma_{110}\hat{\sigma}_x + \gamma_{210}\hat{\sigma}_y + \gamma_{310}\hat{\sigma}_z)\hat{k}_x + (\gamma_{101}\hat{\sigma}_x + \gamma_{201}\hat{\sigma}_y + \gamma_{301}\hat{\sigma}_z)\hat{k}_y$$
(6)

and

$$\hat{H}_{SO}^{(3)} = (\gamma_{130}\hat{\sigma}_x + \gamma_{230}\hat{\sigma}_y + \gamma_{330}\hat{\sigma}_z)\hat{k}_x^3 + (\gamma_{121}\hat{\sigma}_x + \gamma_{221}\hat{\sigma}_y + \gamma_{321}\hat{\sigma}_z)\hat{k}_x^2\hat{k}_y + (\gamma_{112}\hat{\sigma}_x + \gamma_{212}\hat{\sigma}_y + \gamma_{312}\hat{\sigma}_z)\hat{k}_x\hat{k}_y^2 + (\gamma_{103}\hat{\sigma}_x + \gamma_{203}\hat{\sigma}_y + \gamma_{303}\hat{\sigma}_z)\hat{k}_y^3$$
(7)

are the generalized k-linear and k-cubic SOC contributions, respectively.

To obtain the general condition for realizing a collinear SOF, we calculate the commutator of the Hamiltonian (5) with the operator (2):

$$[\hat{H}, \hat{\Sigma}] = i\hbar \left(\sum_{a=0}^{1} \hat{k}_{x}^{a} \hat{k}_{y}^{1-a} \middle| \begin{array}{ccc} \hat{\sigma}_{x} & \hat{\sigma}_{y} & \hat{\sigma}_{z} \\ \gamma_{1, a, 1-a} & \gamma_{2, a, 1-a} & \gamma_{3, a, 1-a} \\ n_{x} & n_{y} & n_{z} \end{array} \right) \\ + \sum_{j=0}^{3} \hat{k}_{x}^{j} \hat{k}_{y}^{3-j} \middle| \begin{array}{ccc} \hat{\sigma}_{x} & \hat{\sigma}_{y} & \hat{\sigma}_{z} \\ \gamma_{1, j, 3-j} & \gamma_{2, j, 3-j} & \gamma_{3, j, 3-j} \\ n_{x} & n_{y} & n_{z} \end{array} \right) \right).$$

$$(8)$$

The commutator (8) vanishes if the following equalities are satisfied:

$$(\boldsymbol{\sigma} \cdot [\boldsymbol{\gamma}_{01} \times \mathbf{n}]) = (\boldsymbol{\sigma} \cdot [\boldsymbol{\gamma}_{10} \times \mathbf{n}]) = \hat{\mathbf{0}}, \quad (9)$$

$$(\boldsymbol{\sigma} \cdot [\boldsymbol{\gamma}_{03} \times \mathbf{n}]) = (\boldsymbol{\sigma} \cdot [\boldsymbol{\gamma}_{12} \times \mathbf{n}]) = (\boldsymbol{\sigma} \cdot [\boldsymbol{\gamma}_{21} \times \mathbf{n}])$$
$$= (\boldsymbol{\sigma} \cdot [\boldsymbol{\gamma}_{30} \times \mathbf{n}]) = \hat{\mathbf{0}}.$$
(10)

Here,

$$\boldsymbol{\gamma}_{01} = \{ \gamma_{101}, \gamma_{201}, \gamma_{301} \}, \quad \boldsymbol{\gamma}_{10} = \{ \gamma_{110}, \gamma_{210}, \gamma_{310} \},$$

$$\boldsymbol{\gamma}_{03} = \{ \gamma_{103}, \gamma_{203}, \gamma_{303} \}, \quad \boldsymbol{\gamma}_{12} = \{ \gamma_{112}, \gamma_{212}, \gamma_{312} \},$$

$$\boldsymbol{\gamma}_{21} = \{ \gamma_{121}, \gamma_{221}, \gamma_{321} \}, \quad \boldsymbol{\gamma}_{30} = \{ \gamma_{130}, \gamma_{230}, \gamma_{330} \} \quad (11)$$

are six symbolic vectors constructed from the SOC parameters.

It is possible to find components of a unit vector **n**, satisfying the condition (9), if the cross product of the vectors $\boldsymbol{\gamma}_{10}$ and $\boldsymbol{\gamma}_{01}$ is zero:

$$[\boldsymbol{\gamma}_{10} \times \boldsymbol{\gamma}_{01}] = \boldsymbol{0}. \tag{12}$$

In this case, the vector **n** defines the conserved spin operator (2) and also determines the direction of the collinear SOF. Let us note that condition (12) defines the possibility of formation of the persistent spin helix, when the **k**-cubic terms are omitted [27].

In general, the collinearity of SOF is destroyed due to the cubic SOC terms (7). However, the SOF remains collinear even in the presence of such terms in some exceptional cases, when the six vectors (11) are either pairwise collinear or null vectors. After the renaming $\boldsymbol{\gamma}_{01} \equiv \boldsymbol{\xi}_1$, $\boldsymbol{\gamma}_{10} \equiv \boldsymbol{\xi}_2$, $\boldsymbol{\gamma}_{03} \equiv \boldsymbol{\xi}_3$, $\boldsymbol{\gamma}_{12} \equiv \boldsymbol{\xi}_4$, $\boldsymbol{\gamma}_{21} \equiv \boldsymbol{\xi}_5$, and $\boldsymbol{\gamma}_{30} \equiv \boldsymbol{\xi}_6$, this condition can be formulated as

$$f_3 = \frac{1}{2} \sum_{i,j=1}^{6} |[\boldsymbol{\xi}_i \times \boldsymbol{\xi}_j]|^2 = 0.$$
(13)

Analogously, for the most general case when the SOC part of the 2D Hamiltonian contains odd in **k** SOC terms up to 2n + 1 order [see Eqs. (3) and (4)] a similar to Eqs. (12) and (13) condition of existence of a conserved spin operator (2) can be obtained. Namely, $\hat{H}_{SO}^{(2j+1)}$ contains $3 \times 2(j+1) = 6(j+1)$ terms. In total, the Hamiltonian (3) is characterized by 3(n+1)(n+2) SOC parameters $\gamma_{s,t,2j+1-t}$, which form (n+1)(n+2) symbolic SOC vectors ξ_i , $i = \overline{1, (n+1)(n+2)}$. It is convenient to introduce a function

$$f_{2n+1} = \frac{1}{2} \sum_{i,j=1}^{(n+1)(n+2)} |[\boldsymbol{\xi}_i \times \boldsymbol{\xi}_j]|^2,$$
(14)

which takes only non-negative values. A conserved spin operator (2) exists if the condition $f_{2n+1} = 0$ is satisfied. In particular, for n = 0 and n = 1 it is reduced to conditions (12) and (13), respectively.

In Secs. IV and V, we apply the conditions (12) and (13) to ZB and wurtzite QWs with different growth directions and identify among them ones in which the collinear SOF can

be realized in the presence of only the **k**-linear and both the **k**-linear and **k**-cubic SOC terms.

III. THE EFFECTIVE 2D DRESSELHAUS HAMILTONIAN OF AN ARBITRARILY ORIENTED ZINC-BLENDE QW: COMPUTATION OF THE COMPLETE SET OF THE SOC PARAMETERS

Let us begin with the full-zone tight-binding SOC Hamiltonian describing the lowest conduction band in III-V bulk semiconductors belonging to T_d point group symmetry [29]:

$$\begin{aligned} \hat{H}_{\text{bulk}} &= E_0 \bigg[\hat{\sigma}_{z_1} \bigg(\cos\left(\frac{k_{x_1}a}{2}\right) - \cos\left(\frac{k_{y_1}a}{2}\right) \bigg) \sin\left(\frac{k_{z_1}a}{2}\right) \\ &+ \hat{\sigma}_{y_1} \bigg(\cos\left(\frac{k_{z_1}a}{2}\right) - \cos\left(\frac{k_{x_1}a}{2}\right) \bigg) \sin\left(\frac{k_{y_1}a}{2}\right) \\ &+ \hat{\sigma}_{x_1} \bigg(\cos\left(\frac{k_{y_1}a}{2}\right) - \cos\left(\frac{k_{z_1}a}{2}\right) \bigg) \sin\left(\frac{k_{x_1}a}{2}\right) \bigg]. \end{aligned}$$

$$(15)$$

Here, E_0 is a constant with energy dimension, *a* is the lattice constant, x_1 , y_1 , and z_1 are cubic axes, i.e., $x_1||[100]$, $y_1||[010]$, $z_1||[001]$. To derive the effective 2D spin Hamiltonian containing all SOC terms up to the third order in **k** compatible with the crystal symmetry, it is necessary to expand the Hamiltonian (15) in a power series about the Γ point and keep all terms of up to the fifth order in **k**:

$$\begin{aligned} \hat{H}_{D}^{\text{bulk}} &= \gamma_{0} \left(\hat{\sigma}_{x_{1}} \hat{k}_{x_{1}} \left(\hat{k}_{y_{1}}^{2} - \hat{k}_{z_{1}}^{2} \right) + \hat{\sigma}_{y_{1}} \hat{k}_{y_{1}} \left(\hat{k}_{z_{1}}^{2} - \hat{k}_{x_{1}}^{2} \right) \right. \\ &\quad + \hat{\sigma}_{z_{1}} \hat{k}_{z_{1}} \left(\hat{k}_{x_{1}}^{2} - \hat{k}_{y_{1}}^{2} \right) \right) \\ &\quad - \frac{a^{2} \gamma_{0}}{48} \left(\hat{\sigma}_{x_{1}} \hat{k}_{x_{1}} \left(\hat{k}_{y_{1}}^{2} - \hat{k}_{z_{1}}^{2} \right) \left(\hat{K}^{2} + \hat{k}_{x_{1}}^{2} \right) \right. \\ &\quad + \hat{\sigma}_{y_{1}} \hat{k}_{y_{1}} \left(\hat{k}_{z_{1}}^{2} - \hat{k}_{x_{1}}^{2} \right) \left(\hat{K}^{2} + \hat{k}_{y_{1}}^{2} \right) \\ &\quad + \hat{\sigma}_{z_{1}} \hat{k}_{z_{1}} \left(\hat{k}_{x_{1}}^{2} - \hat{k}_{y_{1}}^{2} \right) \left(\hat{K}^{2} + \hat{k}_{z_{1}}^{2} \right) \end{aligned}$$
(16)

where $\hat{K}^2 = \hat{k}_{x_1}^2 + \hat{k}_{y_1}^2 + \hat{k}_{z_1}^2$ and the **k**-cubic SOC terms on the right-hand side of the expression (16) form the well-known Dresselhaus Hamiltonian [32] with only one independent constant $\gamma_0 = -a^3 E_0/16$.

It is convenient to rotate the coordinate system such that the z axis of the transformed system is aligned with the QW growth direction, which is defined by the unit vector $\{\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\}$, where θ and φ are polar and azimuthal angles, respectively. The operators $\hat{\mathbf{k}}_1$ and $\hat{\sigma}_1$ in the initial coordinate system are connected with the operators $\hat{\mathbf{k}}$ and $\hat{\sigma}$ in the transformed system as $\hat{\mathbf{k}}_1 = M\hat{\mathbf{k}}, \hat{\sigma}_1 = M\hat{\sigma}$ via the matrix

$$M = \begin{vmatrix} M_{11} & M_{12} & M_{13} \\ M_{12} & M_{22} & M_{23} \\ -M_{13} & -M_{23} & M_{33} \end{vmatrix}$$
(17)

with elements

$$M_{11} = \cos^2 \varphi \cos \theta + \sin^2 \varphi,$$

$$M_{12} = (\cos \theta - 1) \sin \varphi \cos \varphi,$$

$$M_{13} = \sin \theta \cos \varphi, \quad M_{22} = \cos^2 \varphi + \sin^2 \varphi \cos \theta,$$

$$M_{23} = \sin \theta \sin \varphi, \quad M_{33} = \cos \theta.$$

(18)

TABLE I. Parameters R_{abc} and ρ_{abc} of 2D Dresselhaus Hamiltonian \hat{H}_D^{2D} as functions of matrix elements Eq. (18).

Parameters of $\hat{H}_D^{(1)}$

$$\begin{split} & \frac{1}{R_{100}} = -R_{200} = [k_1^2] [W_{11}^2 (W_{12}^2 - W_{12}^2) + M_{11}^2 (W_{12}^2 - W_{12}^2)] + M_{12}^2 (W_{12}^2 - W_{12}^2)] - 2M_{11} M_{23} (M_{11} + M_{13})] \\ & + M_{23} [M_{11} (W_{11}^2 - W_{12}^2) + 2M_{11} (M_{12} M_{23} - M_{11} M_{11})] + M_{22} [M_{12} (W_{12}^2 - W_{12}^2) - 2M_{11} M_{23} (M_{11} + M_{13})] \\ & + M_{23} [M_{11} (W_{11} (W_{12}^2 - W_{12}^2) + 2M_{23} (M_{12} M_{22} - M_{11} M_{11})] + M_{22} [M_{12} (W_{11}^2 - W_{12}^2) - 2M_{11} M_{23} (M_{11} + M_{13})] \\ & + M_{12} [M_{11} (M_{11} (W_{12}^2 - W_{12}^2) + 2M_{13} (M_{21}^2 - W_{12}^2) + M_{12} M_{22} (W_{11}^2 - W_{11}^2) - 2M_{22} (M_{22} M_{22} + M_{22} M_{23})] \\ & + M_{12} [M_{21} (M_{11}^2 - W_{12}^2) + M_{22} M_{23} (M_{11}^2 - M_{12}^2) + M_{23} (M_{11}^2 - M_{12}^2)] \\ & - R_{00} = [k_1^2] [M_{11}^2 (M_{12}^2 - M_{12}^2) + M_{22} M_{23} (M_{12}^2 - M_{12}^2)]] \\ & - R_{00} = [k_1^2] [M_{11}^2 (M_{12}^2 - M_{12}^2) + M_{22} M_{23} (M_{11}^2 - M_{12}^2) + M_{12} M_{23} (M_{11}^2 - M_{12}^2)] \\ & - R_{00} = [k_1^2] [M_{11}^2 (M_{12}^2 - M_{12}^2) + M_{12}^2 M_{23} (M_{12}^2 - M_{12}^2)] + M_{13} M_{13} (M_{12}^2 - M_{12}^2)] \\ & - R_{00} = [k_1^2] [M_{11} (M_{12} (M_{12}^2 - M_{12}^2) + M_{12} M_{23} (M_{12}^2 - M_{23}^2)] + M_{13} M_{13} (M_{12}^2 - M_{12}^2)] \\ & + M_{13} M_{13} (M_{12}^2 - M_{12}^2) (M_{12} - M_{11} M_{23} + M_{13} M_{13} (M_{12}^2 - M_{23}^2)] + M_{13} M_{13} (M_{12}^2 - M_{23}^2)] \\ & + M_{13} M_{13} (M_{12}^2 - M_{12}^2) (M_{12} - M_{11} M_{13} M_{13} (M_{12}^2 - M_{23}^2)] (M_{12} M_{13} - M_{13} M_{13} M_{13} + M_{13} M_{13} (M_{12}^2 - M_{13}^2)] (M_{12} M_{13} - M_{13} M_{13} M_{13} M_{13} + M_{13} M_{13} M_{13} M_{13} + M_{13} M_{13} M_{13} M_{13} M_{13} + M_{13} M_{13}$$

TABLE I. (Continued.)

$$\begin{split} \rho_{230} &= 2 \{k_2^2\} \Big[M_{11}^2 (M_{11}M_{12} (M_{23}^2 - M_{33}^2) - 3M_{12}M_{22} (M_{13}^2 + M_{23}^2) + 3M_{13}M_{23} (M_{12}^2 + M_{33}^2) - 2M_{11}M_{13}M_{23} (M_{22}^2 + M_{33}) \\ &+ 6M_{12}M_{13} (M_{12}M_{23} + M_{13}M_{33}) + M_{12}^2 (M_{12}M_{22} (M_{33}^2 - M_{13}^2) + 3M_{11}M_{12} (M_{13}^2 + M_{23}^2) - 3M_{13}M_{23} (M_{23}^2 + M_{33}^2) \\ &+ 3M_{12}M_{22} (M_{23}^2 + M_{33}^2) + 2M_{13}M_{33} (M_{12}M_{13} - M_{22}M_{23} (M_{11} + M_{33})) + M_{13}^2 (M_{13}M_{23} (M_{12}^2 - M_{13}^2) - 3M_{11}M_{12} (M_{13}^2 + M_{23}^2) \\ &+ 3M_{12}M_{22} (M_{23}^2 + M_{33}^2) + 2M_{13}M_{33} (M_{12}M_{13} - M_{22}M_{23}) + 6M_{23}M_{31} (M_{12}M_{23} - M_{11}M_{13})) \Big], \\ \rho_{221} &= 6 \{k_2^2] \Big[M_{12}^2 (M_{13}^2 - M_{13}^2) + M_{23}^2 (M_{11}^2 + M_{13}^2) - M_{23}^2 (M_{11}^2 + M_{13}^2) + M_{22}^2 (-M_{13}^2 (M_{11}^2 + M_{12}^2) + M_{23}^2 (M_{13}^2 - M_{11}^2) \\ &+ M_{33}^2 (M_{12}^2 - M_{13}^2) + M_{23}^2 (M_{11}^2 + M_{13}^2) - M_{23}^2 (M_{12}^2 + M_{13}^2) + M_{23}^2 (M_{11}^2 - M_{12}^2) + 4M_{11}M_{12}^2 M_{13} (M_{12}M_{23} - M_{11}^2) \\ &- 4M_{12}M_{13}M_{22}^2 M_{23}^2 (M_{11} + M_{33}) + 4M_{13}M_{23}^2 M_{33} (M_{12}M_{23} - M_{11}) \Big], \\ \rho_{122} &= 6 \{k_2^2] \Big[M_{11}M_{12} (M_{13}^2 (M_{23}^2 - M_{22}^2) + M_{23}^2 (M_{12}^2 - M_{23}^2) + M_{33}^2 (M_{22}^2 - M_{12}^2) \Big] + 4M_{11}M_{12}^2 M_{13} (M_{12}^2 - M_{23}^2) \\ &- 4M_{33}^2 (M_{12}^2 - M_{23}^2) \Big] + M_{13}M_{23} (M_{13}^2 M_{23}^2 - M_{22}^2) + M_{33}^2 (M_{22}^2 - M_{23}^2) \Big] + 2M_{13}M_{23} (M_{12}^2 - M_{23}^2) \Big] \\ \rho_{203} &= 2 \{k_2^2] \Big[M_{11}^2 M_{13} (M_{12}^2 - M_{23}^2) \Big] + M_{13}M_{21} (M_{13}^2 - M_{23}^2) + M_{23}^2 (M_{13}^2 - M_{23}^2) \Big] + M_{13}^2 (M_{13}^2 - M_{23}^2) \Big] + M_{13}M_{23} (M_{12}^2 - M_{23}^2) \\ + 2M_{13}M_{33} (M_{12}^2 - M_{23}^2) \Big] + M_{13}^2 (M_{13}^2 - M_{23}^2) + M_{13}^2 (M_{13}^2 - M_{23}^2) \Big] \Big] \\ \rho_{303} &= 2 \{k_2^2] \Big[M_{11}M_{13} (M_{11}^2 - M_{23}^2) + M_{12}^2 (M_{13}^2 - M_{23}^2) + M_{12}^2 (M_{13}^2 - M_{23}^2) + M_{12}^2 (M_{13}^2 - M_{23}^2) \Big] \\ + M_{13}^2 (M_{23}^$$

For the lowest size quantization subband in the symmetric QW, the effective 2D SOC Hamiltonian can be obtained via averaging of the Hamiltonian (16) along the growth direction (the *z* axis) [26]. We have $\langle k_z \rangle = \langle k_z^3 \rangle = \langle k_z^5 \rangle = 0$, but $\langle k_z^2 \rangle \neq 0$ and $\langle k_z^4 \rangle \neq 0$ defined by the potential profile. In particular, in an infinite quantum square well of width *d*, one has $\langle k_z^n \rangle = (\frac{1+(-1)^n}{2})(\pi/d)^n$ for any integer *n*. Replacing $\hat{\mathbf{k}}_1 = M\hat{\mathbf{k}}$ and $\hat{\boldsymbol{\sigma}}_1 = M\hat{\boldsymbol{\sigma}}$ in Eq. (16) together with averaging along the *z* direction yields 2D Dresselhaus Hamiltonian

$$\hat{H}_D^{2D} = \hat{H}_D^{(1)} + \hat{H}_D^{(3)}.$$
(19)

The **k**-linear $\hat{H}_D^{(1)}$ and **k**-cubic $\hat{H}_D^{(3)}$ parts of the Hamiltonian (19) contain six and 12 SOC parameters $\{\beta_{abc}^{(1)}\}$ and $\{\beta_{abc}^{(3)}\}$, respectively, which can be written in the same way as $\beta_{abc}^{(j)} = \gamma_0(R_{abc} - a^2\rho_{abc}/48)$. Expressions for R_{abc} and ρ_{abc} are listed in Table I.

The other contribution to the SOC Hamiltonian is connected with the structure inversion asymmetry and is described by the well-known \mathbf{k} -linear Rashba term [33,34]:

$$\hat{H}_{R}^{(1)} = \alpha_{210}(\hat{\sigma}_{y}\hat{k}_{x} - \hat{\sigma}_{x}\hat{k}_{y}), \qquad (20)$$

where the Rashba parameter α_{210} is proportional to the potential gradient along the growth direction of the QW and,

therefore, can be varied experimentally [35] (for instance, by means of external electric field). The Rashba term (20) is independent of the growth direction and is invariant under rotations in the plane of the QW. For correct investigation of possibilities for realization of the collinear SOF in asymmetric ZB QWs in the presence of the **k**-cubic SOC terms, it is also necessary to take into account the **k**-cubic Rashba SOC contributions. In our analysis of ZB QWs presented below, we employ the expressions for the **k**-cubic Rashba SOC terms derived by Cartoixa *et al.* in Ref. [29].

TABLE II. Correspondence between growth orientationdependent x, y, z labels for different ZB 2DES and crystallographic directions.

	(001)	(110)	(111)	(113)	(013)
x	[100]	[110]	[112]	[110]	[100]
y	[010]	[001]	[110]	[332]	[031]
z	[001]	[110]	[111]	[113]	[013]

TABLE III. Nonzero SOC parameters of the Hamiltonians $\hat{H}_D^{(1)}$ and $\hat{H}_D^{(3)}$ corresponding to ZB QWs with different growth directions.

$$\begin{split} & [001] \\ \beta_{201}^{(1)} = -\beta_{110}^{(1)} = \gamma_0 \left(\frac{\pi}{d}\right)^2 \left[1 - \frac{1}{48} \left(\frac{\pi a}{d}\right)^2\right], \quad \beta_{112}^{(3)} = -\beta_{221}^{(3)} = \gamma_0, \quad \beta_{130}^{(3)} = -\beta_{203}^{(3)} = \frac{\gamma_0}{24} \left(\frac{\pi a}{d}\right)^2. \\ & [113] \\ \beta_{101}^{(1)} = -\frac{6\sqrt{11}}{121} \gamma_0 \left(\frac{\pi}{d}\right)^2 \left[1 - \frac{5}{132} \left(\frac{\pi a}{d}\right)^2\right], \quad \beta_{210}^{(1)} = -\frac{42\sqrt{11}}{121} \gamma_0 \left(\frac{\pi}{d}\right)^2 \left[1 - \frac{9}{306} \left(\frac{\pi a}{d}\right)^2\right], \quad \beta_{310}^{(1)} = \frac{8\sqrt{22}}{121} \gamma_0 \left(\frac{\pi}{d}\right)^2 \left[1 - \frac{7}{131} \left(\frac{\pi a}{d}\right)^2\right], \\ \beta_{103}^{(3)} = \frac{15\sqrt{11}}{242} \gamma_0 \left[1 - \frac{29}{660} \left(\frac{\pi a}{d}\right)^2\right], \quad \beta_{121}^{(3)} = -\frac{3\sqrt{11}}{222} \gamma_0 \left[1 - \frac{3}{44} \left(\frac{\pi a}{d}\right)^2\right], \quad \beta_{212}^{(3)} = -\frac{15\sqrt{11}}{242} \gamma_0 \left[1 - \frac{34}{4} \left(\frac{\pi a}{d}\right)^2\right], \\ \beta_{230}^{(3)} = \frac{3\sqrt{11}}{222} \gamma_0 \left[1 + \frac{7}{132} \left(\frac{\pi a}{d}\right)^2\right], \quad \beta_{330}^{(3)} = \frac{\gamma_0}{\sqrt{22}} \left[1 - \frac{1}{34} \left(\frac{\pi a}{d}\right)^2\right], \quad \beta_{312}^{(3)} = -\frac{49\sqrt{22}}{242} \gamma_0 \left[1 - \frac{23}{539} \left(\frac{\pi a}{d}\right)^2\right]. \\ \\ \beta_{310}^{(1)} = \frac{\gamma_0}{2} \left(\frac{\pi}{d}\right)^2 \left[1 - \frac{1}{96} \left(\frac{\pi a}{d}\right)^2\right], \quad \beta_{330}^{(3)} = -\frac{\gamma_0}{22} \left[1 + \frac{1}{48} \left(\frac{\pi a}{d}\right)^2\right], \quad \beta_{312}^{(3)} = \gamma_0 \left[1 - \frac{13}{128} \left(\frac{\pi a}{d}\right)^2\right]. \\ \\ \beta_{210}^{(1)} = -\beta_{101}^{(1)} = \frac{2}{\sqrt{3}} \gamma_0 \left(\frac{\pi}{d}\right)^2 \left[1 - \frac{1}{36} \left(\frac{\pi a}{d}\right)^2\right], \quad \beta_{230}^{(3)} = \beta_{212}^{(3)} = -\beta_{103}^{(3)} = \frac{\sqrt{3}}{6} \gamma_0 \left[1 + \frac{1}{12} \left(\frac{\pi a}{d}\right)^2\right], \quad \beta_{303}^{(3)} = -\sqrt{6} \gamma_0 /2. \\ \\ \hline \end{split}$$

IV. THE COLLINEAR SOF IN ZINC-BLENDE QWS OF DIFFERENT GROWTH DIRECTIONS

Before application of the conditions (12) and (13) to ZB QWs with different growth directions and identification among them that ones, in which the collinear SOF can be realized, let us note that the functional form of the Dresselhaus contributions depends on the orientation of the coordinate axes in the plane of the QW. Typically, an additional rotation around the *z* axis on a certain angle is needed to arrive at the natural orientation of the Dresselhaus 2D Hamiltonian has the simplest form. Correspondence between growth orientation-dependent *x*, *y*, *z* labels for different 2DES and crystallographic directions is given in Table II.

[001] ZB QWs. For [001] QWs we have the well-known **k**-linear Dresselhaus Hamiltonian

$$\hat{H}_D^{(1)\ [001]} = \beta_{201}^{(1)}(\hat{\sigma}_y \hat{k}_y - \hat{\sigma}_x \hat{k}_x), \tag{21}$$

with the Dresselhaus parameter $\beta_{201}^{(1)} = \gamma_0 (\frac{\pi}{d})^2 [1 - \frac{1}{48} (\frac{\pi a}{d})^2]$, and the **k**-cubic Hamiltonian

$$\hat{H}_{D}^{(3)\ [001]} = \beta_{112}^{(3)} \hat{k}_x \hat{k}_y (\hat{\sigma}_x \hat{k}_y - \hat{\sigma}_y \hat{k}_x) + \beta_{130}^{(3)} (\hat{\sigma}_x \hat{k}_x^3 - \hat{\sigma}_y \hat{k}_y^3),$$
(22)

with the SOC parameters $\beta_{112}^{(3)} = \gamma_0$ and $\beta_{130}^{(3)} = \frac{\gamma_0}{24} (\frac{\pi a}{d})^2$. For convenience all nonzero SOC parameters of $\hat{H}_D^{(1)}[^{001}]$ and $\hat{H}_D^{(3)}[^{001}]$ are also collected in Table III. The sum of the Hamiltonians (21) and (22) reproduces the Dresselhaus Hamiltonian for [001] ZB QWs derived in Ref. [29]. Hamiltonian (21) and the first term in the right-hand side of expression (22) recover the conventional **k**-linear and **k**-cubic Dresselhaus contributions, respectively [24,26]. The remaining term in the righthand side of expression (22) appears from averaging of the fifth order in **k** terms included in the bulk Hamiltonian (16). Although this term is small enough $(\beta_{130}^{(3)}/\beta_{112}^{(3)} \propto (a/d)^2 \ll 1)$, it is necessary for accurate investigation of possibilities for realization of the collinear SOF in the presence of the **k**-cubic SOC terms.

For symmetric [001] ZB QWs the cross product of two SOC vectors $\boldsymbol{\gamma}_{10} = \beta_{201}^{(1)} \{-1, 0, 0\}$ and $\boldsymbol{\gamma}_{01} = \beta_{201}^{(1)} \{0, 1, 0\}$ is not the null vector. Hence, the SOF is not collinear in such QWs even if only the **k**-linear SOC terms are taken into account. For asymmetric QWs with the same orientation, the SOC part of the effective 2D Hamiltonian should be complemented by the Rashba SOC contributions. The **k**-linear Rashba SOC term is defined by the Hamiltonian (20), while the complete set of the **k**-cubic Rashba SOC contributions for [001] ZB QWs is described by the following expression [29]:

$$\hat{H}_{R}^{(3)\ [001]} = \alpha_{103} \big(\hat{\sigma}_{x} \hat{k}_{y}^{3} - \hat{\sigma}_{y} \hat{k}_{x}^{3} \big) + \alpha_{121} \hat{k}_{x} \hat{k}_{y} (\hat{\sigma}_{x} \hat{k}_{x} - \hat{\sigma}_{y} \hat{k}_{y}).$$
(23)

For the first two SOC vectors, we have $\boldsymbol{\gamma}_{10} = \{-\beta_{201}^{(1)}, \alpha_{210}, 0\}$ and $\boldsymbol{\gamma}_{01} = \{-\alpha_{210}, \beta_{201}^{(1)}, 0\}$. In this case, the condition $[\boldsymbol{\gamma}_{10} \times \boldsymbol{\gamma}_{01}] = \mathbf{0}$ is satisfied when $\alpha_{210} = \pm \beta_{201}^{(1)}$. Next, from expressions (20)–(23) one can find that

$$\boldsymbol{\gamma}_{30} = \{ \beta_{130}^{(3)}, -\alpha_{103}, 0 \}, \quad \boldsymbol{\gamma}_{21} = \{ \alpha_{121}, -\beta_{112}^{(3)}, 0 \}, \\ \boldsymbol{\gamma}_{12} = \{ \beta_{112}^{(3)}, -\alpha_{121}, 0 \}, \quad \boldsymbol{\gamma}_{03} = \{ \alpha_{103}, -\beta_{130}^{(3)}, 0 \},$$
(24)

and there are two cases when the condition $f_3 = 0$ is satisfied:

$$\alpha_{210} = \beta_{201}^{(1)}, \quad \alpha_{103} = \beta_{130}^{(3)}, \quad \alpha_{121} = \beta_{112}^{(3)}, \quad (25)$$

or

$$\alpha_{210} = -\beta_{201}^{(1)}, \quad \alpha_{103} = -\beta_{130}^{(3)}, \quad \alpha_{121} = -\beta_{112}^{(3)}.$$
 (26)

Relations (25) and (26) correspond to the situations when the SOF is collinear to the $[\bar{1}10]$ and [110] directions, respectively. The above finding supplements the relevant result of Ref. [25]. We note again that although the **k**-cubic Rashba terms are expected to be small enough in comparison with the **k**-linear Rashba terms their inclusion is necessary for correct investigation of the possibilities for realization of the collinear

SOF in asymmetric ZB QWs in the presence of the **k**-cubic SOC terms.

[113] ZB QWs. For this growth direction ($\theta = \arccos(3/\sqrt{11}), \varphi = \pi/4$) we have

$$\hat{H}_D^{(1) [113]} = \beta_{101}^{(1)} \hat{\sigma}_x \hat{k}_y + \beta_{210}^{(1)} \hat{\sigma}_y \hat{k}_x + \beta_{310}^{(1)} \hat{\sigma}_z \hat{k}_x, \qquad (27)$$

and

$$\hat{H}_{D}^{(3)\ [113]} = \beta_{103}^{(3)} \hat{\sigma}_{x} \hat{k}_{y}^{3} + \beta_{230}^{(3)} \hat{\sigma}_{y} \hat{k}_{x}^{3} + \left(\beta_{121}^{(3)} \hat{\sigma}_{x} \hat{k}_{x} + \beta_{212}^{(3)} \hat{\sigma}_{y} \hat{k}_{y}\right) \hat{k}_{x} \hat{k}_{y} + \left(\beta_{330}^{(3)} \hat{k}_{x}^{2} + \beta_{312}^{(3)} \hat{k}_{y}^{2}\right) \hat{\sigma}_{z} \hat{k}_{x}$$
(28)

with the SOC parameters $\{\beta_{abc}^{(1)}\}\$ and $\{\beta_{abc}^{(3)}\}\$ from Table III. The Hamiltonian (27) implies that for symmetric [113] ZB QWs $\boldsymbol{\gamma}_{10} = \{0, \beta_{210}^{(1)}, \beta_{310}^{(1)}\}, \boldsymbol{\gamma}_{01} = \{\beta_{101}^{(1)}, 0, 0\}\$, and the collinear SOF cannot be realized in such QWs. In asymmetric QWs with the same orientation the cross product of two SOC vectors $\boldsymbol{\gamma}_{10} = \{0, \beta_{210}^{(1)} + \alpha_{210}^{(1)}, \beta_{310}^{(1)}\}\$ and $\boldsymbol{\gamma}_{01} = \{\beta_{101}^{(1)} - \alpha_{210}^{(1)}, 0, 0\}\$ is zero if

$$\alpha_{210}^{(1)} = \beta_{101}^{(1)} = -\frac{6\sqrt{11}}{121}\gamma_0 \left(\frac{\pi}{d}\right)^2 \left[1 - \frac{5}{132} \left(\frac{\pi a}{d}\right)^2\right].$$
 (29)

In this case, $\boldsymbol{\gamma}_{01} = \boldsymbol{0}$.

Before we analyze the influence of the **k**-cubic SOC terms let us note that ZB structure based (113)-oriented 2DES belongs to the symmetry point group C_s , which contains only two elements, the identity and one mirror reflection plane, being normal to the 2DES plane [30]. It is easy to see that the inclusion of the Rashba SOC does not reduce the symmetry with respect to the case when only the Dresselhaus SOC is taken into account. Hence, the functional form of the **k**-cubic SOC Hamiltonian for asymmetric ZB [113] QWs coincides with the Hamiltonian (28), in which each of the SOC parameter $\beta_{abc}^{(3)}$ should be replaced by the sum $\beta_{abc}^{(3)} + \alpha_{abc}^{(3)}$, where corrections { $\alpha_{abc}^{(3)}$ } describe renormalization of the Dresselhaus parameters due to the **k**-cubic Rashba SOC. It yields the following four SOC vectors:

$$\begin{aligned} \boldsymbol{\gamma}_{30} &= \left\{ 0, \, \beta_{230}^{(3)} + \alpha_{230}^{(3)}, \, \beta_{330}^{(3)} + \alpha_{330}^{(3)} \right\}, \\ \boldsymbol{\gamma}_{21} &= \left\{ \beta_{121}^{(3)} + \alpha_{121}^{(3)}, \, 0, \, 0 \right\}, \\ \boldsymbol{\gamma}_{12} &= \left\{ 0, \, \beta_{212}^{(3)} + \alpha_{212}^{(3)}, \, \beta_{312}^{(3)} + \alpha_{312}^{(3)} \right\}, \\ \boldsymbol{\gamma}_{03} &= \left\{ \beta_{103}^{(3)} + \alpha_{103}^{(3)}, \, 0, \, 0 \right\}. \end{aligned}$$
(30)

Thus, for realization of the collinear SOF in [113] ZB QWs in the presence of both the **k**-linear and **k**-cubic SOC contributions it necessary to vanish the function f_3 with the vectors (30) complemented by the two vectors $\boldsymbol{\gamma}_{10} = \{0, \beta_{210}^{(1)} + \beta_{101}^{(1)}, \beta_{310}^{(1)}\}$ and $\boldsymbol{\gamma}_{01} = \boldsymbol{0}$ [we use here relation (29)]. One can find, however, that experimental adjustment of the SOC parameters for satisfaction of the condition $f_3 = 0$ seems to be hardly realizable.

[110] ZB QWs. QWs on [110]-oriented GaAs substrates have attracted considerable attention due to their extraordinary spin dephasing, which can reach several hundreds of nanoseconds (see the review [30] and references therein). In a [110] symmetric QW of this type the SOF points into the growth direction [26]. Therefore, spins oriented along this direction do not precess and the Dyakonov-Perel spin relaxation mechanism, which is based on the spin precession in the effective magnetic field, is suppressed. For [110] ZB QWs the sum of the **k**-linear and **k**-cubic 2D Dresselhaus Hamiltonians has the simple form:

$$\hat{H}_{D}^{(1)[110]} + \hat{H}_{D}^{(3)[110]} = \hat{\sigma}_{z}\hat{k}_{x} \left(\beta_{310}^{(1)} + \beta_{330}^{(3)}\hat{k}_{x}^{2} + \beta_{312}^{(3)}\hat{k}_{y}^{2}\right), \quad (31)$$

with three nonzero SOC parameters $\beta_{310}^{(1)}$, $\beta_{330}^{(3)}$, and $\beta_{312}^{(3)}$ (see Table III). Expression (31) implies that the SOF in symmetric [110] ZB QWs is collinear in the presence of both the **k**-linear and **k**-cubic SOC terms. Moreover, this result still holds even when all SOC terms up to an arbitrary odd in **k** order are included. The explicit proof of this statement within our approach is given in the Appendix.

The **k**-linear SOC terms in asymmetric [110] ZB QWs, which have C_s symmetry, are described by the sum of the linear part $\hat{H}_D^{(1)[110]} = \beta_{310}^{(1)} \hat{\sigma}_z \hat{k}_x$ of the Hamiltonian (31) and the Rashba Hamiltonian (20). In this case, we have two SOC vectors $\boldsymbol{\gamma}_{10} = \{0, \alpha_{210}, \beta_{310}^{(1)}\}, \boldsymbol{\gamma}_{01} = \{-\alpha_{210}, 0, 0\}$, and, as a result, the absence of the collinearity of the corresponding SOF.

[111] ZB QWs. Implementation of our computational routine for [111] QWs ($\theta = \arccos(1/\sqrt{3}), \varphi = \pi/4$) leads to the following expressions for the **k**-linear and **k**-cubic Dresselhaus Hamiltonians [29]:

$$\hat{H}_D^{(1)[111]} = \beta_{210}^{(1)}(\hat{\sigma}_y \hat{k}_x - \hat{\sigma}_x \hat{k}_y), \qquad (32)$$

$$\hat{H}_{D}^{(3)[111]} = \beta_{230}^{(3)} (\hat{k}_{x}^{2} + \hat{k}_{y}^{2}) (\hat{\sigma}_{y} \hat{k}_{x} - \hat{\sigma}_{x} \hat{k}_{y}) + \beta_{303}^{(3)} (\hat{k}_{y}^{2} - 3\hat{k}_{x}^{2}) \hat{\sigma}_{z} \hat{k}_{y}, \qquad (33)$$

with the set of the SOC parameters $\{\beta_{abc}^{(1)}\}\$ and $\{\beta_{abc}^{(3)}\}\$, which is shown in Table III. In symmetric [111] ZB QWs the cross product of the first two SOC vectors $\boldsymbol{\gamma}_{10} = \{0, \beta_{210}^{(1)}, 0\}$ and $\boldsymbol{\gamma}_{01} = \{-\beta_{210}^{(1)}, 0, 0\}$ is not zero and the collinear SOF cannot be realized in such QWs.

Next, symmetric [111] ZB QWs transform according to the C_{3v} point group, which consists of the identity, two threefold rotations about the growth axis, and three reflection planes separated by 120° that contain the threefold axes [29]. Analogously to [113] ZB QWs, inclusion of the Rashba SOC does not reduce the symmetry with respect to the case when only the Dresselhaus SOC is taken into account. Therefore, the functional form of the Dresselhaus and the Rashba SOC contributions to the SOC Hamiltonian is the same for [111] ZB QWs. Consequently, the resulting **k**-linear and **k**-cubic parts of the SOC Hamiltonian are described, respectively, by expressions (32) and (33), in which the SOC parameters $\beta_{abc}^{(j)}$ should be replaced by the sum $\beta_{abc}^{(j)} + \alpha_{abc}^{(j)}$, where corrections { $\alpha_{abc}^{(j)}$ }, again, define renormalization of the Dresselhaus parameters due to the Rashba SOC.

In particular, $\gamma_{10} = \gamma_{01} = 0$ and the **k**-linear Dresselhaus and Rashba SOC contributions compensate each other when the condition

$$\alpha_{210} = -\beta_{210}^{(1)} = -\frac{2}{\sqrt{3}}\gamma_0 \left(\frac{\pi}{d}\right)^2 \left[1 - \frac{1}{36}\left(\frac{\pi a}{d}\right)^2\right] \quad (34)$$

is satisfied. The possibilities for realization of the collinear SOF in the presence of the \mathbf{k} -cubic terms are described by the remaining four SOC vectors:

$$\boldsymbol{\gamma}_{30} = \{0, \beta_{230}^{(3)} + \alpha_{230}^{(3)}, 0\}, \boldsymbol{\gamma}_{21} = \{-\beta_{230}^{(3)} + \alpha_{121}^{(3)}, 0, -3\beta_{303}^{(3)} + \alpha_{321}^{(3)}\}, \boldsymbol{\gamma}_{12} = \{0, \beta_{230}^{(3)} + \alpha_{212}^{(3)}, 0\}, \boldsymbol{\gamma}_{03} = \{-\beta_{230}^{(3)} + \alpha_{103}^{(3)}, 0, \beta_{303}^{(3)} + \alpha_{303}^{(3)}\}.$$
(35)

However, for clear conclusions concerning this issue a reliable determination of components of the SOC vectors Eq. (35) or extraction of the SOC parameters $\beta_{abc}^{(j)}$ and $\alpha_{abc}^{(j)}$ with usage of the more complicated computational approaches [36–38] or from experiments is needed.

[013] ZB QWs. We also consider [013] QWs ($\theta = \arccos(3/\sqrt{10}), \varphi = \pi/2$) because of the fact that substrates with this orientation are used for growth of HgTe-based topological insulators [30,39]. For this case, one can find that

$$\hat{H}_D^{(1)[013]} = \beta_{110}^{(1)} \hat{\sigma}_x \hat{k}_x + \beta_{201}^{(1)} \hat{\sigma}_y \hat{k}_y + \beta_{301}^{(1)} \hat{\sigma}_z \hat{k}_y.$$
(36)

Here, the Dresselhaus parameters $\beta_{110}^{(1)}$, $\beta_{201}^{(1)}$, and $\beta_{301}^{(1)}$ (see Table III) define two SOC vectors $\boldsymbol{\gamma}_{10} = \beta_{110}^{(1)} \{1, 0, 0\}$ and $\boldsymbol{\gamma}_{01} = \{0, \beta_{210}^{(1)}, \beta_{301}^{(1)}\}$, which yield $f_1 \neq 0$. In asymmetric [013] ZB QWs inclusion of the Rashba term (20) modifies these vectors as $\boldsymbol{\gamma}_{10} = \{\beta_{110}^{(1)}, \alpha_{210}, 0\}$ and $\boldsymbol{\gamma}_{01} = \{-\alpha_{210}, \beta_{201}^{(1)}, \beta_{301}^{(1)}\}$, but the corresponding SOF still remains noncollinear. Thus, in agreement with the condition obtained in Ref. [25], the collinear SOF cannot be realized in [013] ZB QWs even in the presence of only the **k**-linear Dresselhaus and Rashba SOC contributions.

V. THE COLLINEAR SOF IN WURTZITE 2DES

As was mentioned above, the developed formalism is applicable not only for ZB QWs, but also for the other 2DES that are described by the Hamiltonian (3). Aside from ZB low-dimensional structures, their wurtzite-type (WZ) counterparts have been intensively investigated [9,23,40–47]. In particular, first-principles density-functional theory calculations of the ZnO (1010) surface were performed in Ref. [9]. The authors found that the persistent spin helix can be achieved using a wurtzite (1010) surface or interface with in-plane electric polarization and mirror symmetry. Moreover, experimental investigation of a 2DEG created at the interface of semiconductor/insulator homojunction at the (1010) surface of a Lidoped ZnO microwire indicated the realization of a persistent spin helix in ZnO [23].

In this section, we explore possibilities for realization of the collinear SOF in 2D WZ systems. The SOC Hamiltonian for the conduction electrons in bulk WZ III-V semiconductors has the following form [41,48,49]:

$$\hat{H}_{\text{bulk}}^{WZ} = \left(\alpha_{WZ} + \gamma_{WZ} \left(b\hat{k}_{z_1}^2 - \hat{k}_{x_1}^2 - \hat{k}_{y_1}^2\right)\right) \left(\hat{\sigma}_{x_1}\hat{k}_{y_1} - \hat{\sigma}_{y_1}\hat{k}_{x_1}\right),\tag{37}$$

where $x_1||[11\bar{2}0], y_1||[1\bar{1}00], z_1||[0001]$ (*c*-axis), α_{WZ} and γ_{WZ} are two material-dependent constants. The **k**-cubic Dresselhaus term in the right-hand side of expression (37) is a consequence of the bulk inversion asymmetry of the crystal lattice, while the **k**-linear term occurs in the WZ structure due to the hexagonal *c*-axis and reflects an intrinsic wurtzite structure inversion asymmetry [41]. Correspondingly, the Dresselhaus coefficient γ_{WZ} , together with the material parameter *b*, determines the Dresselhaus contribution, while the coefficient α_{WZ} gives the strength of the WZ intrinsic Rashba-like contribution.

Let us now employ the computational routine presented in Sec. III for calculation of the SOC vectors for various WZ 2DES, which orientation in space is characterized by the unit vector $\mathbf{e}_z = \{\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta\}$ being normal to the 2DEG plane. Rotation of the coordinate system such that the *z* axis of the transformed system is aligned with the vector \mathbf{e}_z is equivalent to the transformation of the operators $\hat{\mathbf{k}}_1$ and $\hat{\sigma}_1$ in the Hamiltonian (37) into the operators $\hat{\mathbf{k}}$ and $\hat{\sigma}$ via the matrix (17). In this section, we restrict our consideration only by the **k**-linear SOC terms (6), which can be derived after averaging of the bulk Hamiltonian (37) along the *z* direction within the lowest conduction subband:

$$\hat{H}_{WZ}^{(1)} = \left(\beta_{110}^{WZ}\hat{\sigma}_x + \beta_{210}^{WZ}\hat{\sigma}_y + \beta_{310}^{WZ}\hat{\sigma}_z\right)\hat{k}_x \\ + \left(\beta_{101}^{WZ}\hat{\sigma}_x + \beta_{201}^{WZ}\hat{\sigma}_y + \beta_{301}^{WZ}\hat{\sigma}_z\right)\hat{k}_y.$$
(38)

Here, the directions of the *x* and *y* axes with respect of the initial coordinate system $Ox_1y_1z_1$ are described by the unit vectors $\mathbf{e}_x = \{\cos^2\varphi\cos\theta + \sin^2\varphi, (\cos\theta - 1)\cos\varphi\sin\varphi, -\sin\theta\cos\varphi\}$ and $\mathbf{e}_y = \{(\cos\theta - 1)\cos\varphi\sin\varphi, \cos^2\varphi + \sin^2\varphi\cos\theta, -\sin\theta\sin\varphi\}$. The SOC parameters of the Hamiltonian (38) are expressed in terms of the spherical angles θ and φ as follows:

$$\begin{aligned} \beta_{201}^{WZ} &= -\beta_{110}^{WZ} = \gamma_{WZ} \langle k_z^2 \rangle \eta(\theta) \cos \theta \sin 2\varphi, \\ \beta_{210}^{WZ} &= -\cos \theta \left(\alpha_{WZ} + \gamma_{WZ} \langle k_z^2 \rangle (b - (2 + \cos 2\varphi)\eta(\theta)) \right) \\ \beta_{310}^{WZ} &= -\sin \theta \sin \varphi \left(\alpha_{WZ} + \gamma_{WZ} \langle k_z^2 \rangle (b - \eta(\theta)) \right), \\ \beta_{101}^{WZ} &= \cos \theta \left(\alpha_{WZ} + \gamma_{WZ} \langle k_z^2 \rangle (b + (\cos 2\varphi - 2)\eta(\theta)) \right), \\ \beta_{301}^{WZ} &= \sin \theta \cos \varphi \left(\alpha_{WZ} + \gamma_{WZ} \langle k_z^2 \rangle (b - \eta(\theta)) \right). \end{aligned}$$
(39)

Here, the definition $\eta(\theta) = (b+1)\sin^2\theta$ is made. The complete set of the SOC terms of higher orders in **k** would be obtained by application of the double group tight-binding formalism [29] to wurtzite 2D systems with the known symmetry.

The collinear SOF is realized for combinations of the parameters, which vanish the function $f_1 = |[\boldsymbol{\gamma}_{10} \times \boldsymbol{\gamma}_{01}]|^2$ constructed from the SOC vectors $\boldsymbol{\gamma}_{10} = \{\beta_{110}^{WZ}, \beta_{210}^{WZ}, \beta_{310}^{WZ}\}$ and $\boldsymbol{\gamma}_{01} = \{\beta_{101}^{WZ}, \beta_{201}^{WZ}, \beta_{301}^{WZ}\}$:

$$f_1 = \cos^2\theta (\Gamma + b - \eta(\theta))^2 (\Gamma + b - 3\eta(\theta))^2, \qquad (40)$$

where $\Gamma = \frac{\alpha_{WZ}}{\gamma_{WZ} \langle k_z^2 \rangle}$. We note that expression (40) does not contain the angle φ .

For the 2DEG planes, which are parallel to the [0001] direction ($\theta = \pi/2$), the Hamiltonian (38) reads as

$$\hat{H}_{WZ}^{(1),\,\theta=\pi/2} = \left(\gamma_{WZ} \langle k_z^2 \rangle - \alpha_{WZ}\right) (\hat{k}_x \sin\varphi - \hat{k}_y \cos\varphi) \hat{\sigma}_z.$$
(41)

	GaAs	GaSb	InAs	InSb
$\overline{\alpha_{WZ}, \mathrm{eV} \cdot \mathrm{\AA}}$	0.1	0.49	0.3	0.71
$\gamma_{WZ}, \ \mathrm{eV} \cdot \mathrm{\AA}^3$	1.92	18.7	132.5	892
b	0.06	-0.04	-1.24	-0.91
Values of d , for which solutions (42) exist, Å	$d \leqslant 13.8$	$3.9 \leqslant d \leqslant 19.4$	$66.0 \leqslant d \leqslant 73.5$	$106.2 \leqslant d \leqslant 111.4$
Values of d , for which solutions (43) exist, Å	$d \leqslant 24.3$	$3.9 \leqslant d \leqslant 33.2$	$47.6 \leqslant d \leqslant 73.5$	$106.2 \leqslant d \leqslant 121.0$

TABLE IV. Values of the QW width *d*, which allow existence of the solutions (42) and (43). Parameters α_{WZ} , γ_{WZ} , and *b* for GaAs, GaSb, InAs, and InSb in wurtzite phase are taken from Ref. [50].

For this type of WZ 2DES, the corresponding SOF is collinear and perpendicular to the 2DEG plane for any value of angle φ . The latter means that the SOF is collinear, for example, in [1010] and [1120] WZ QWs in the presence of only the **k**-linear SOC terms.

After exclusion of the case $\Gamma = -b = 1$ giving the zero SOF, one can find from relation (40) the two series of solutions yielding the collinear SOF:

$$\begin{bmatrix} \theta_1 = \frac{1}{2} \arccos \left(2\xi - 1 \right) \\ \theta_2 = \pi - \frac{1}{2} \arccos \left(2\xi - 1 \right), & \xi \in [0, 1], \quad (42) \end{bmatrix}$$

and

$$\begin{bmatrix} \theta_3 = \frac{1}{2} \arccos\left(\frac{2\xi+1}{3}\right) \\ \theta_4 = \pi - \frac{1}{2} \arccos\left(\frac{2\xi+1}{3}\right), & \xi \in [-2, 1], \quad (43) \end{bmatrix}$$

where $\xi = (1 - \Gamma)/(b + 1)$ is a dimensionless parameter. For both cases the Hamiltonian (38) can be written as

$$\hat{H}_{\text{SOC}}^{(1)} = C_{\text{SOC}}(\mathbf{e}_{\text{2DEG}} \cdot \hat{\mathbf{k}})(\mathbf{e}_{\text{SOF}} \cdot \boldsymbol{\sigma}), \qquad (44)$$

where $\mathbf{e}_{2\text{DEG}}$ is a two-dimensional unit vector laying in the 2DEG plane (apparently, the direction of $\mathbf{e}_{2\text{DEG}}$ coincides with the direction of the so-called "magic" vector [4,24,27]), \mathbf{e}_{SOF} is the unit vector aligned with the collinear SOF, and C_{SOC} is the combination of the SOC parameters defining the strength of the resulting SOF. In particular, for the case (42) these parameters read as

$$C_{\text{SOC}} = 2(\alpha_{WZ} + b\gamma_{WZ} \langle k_z^2 \rangle),$$

$$\mathbf{e}_{\text{2DEG}} = \{\cos\varphi, \sin\varphi\},$$

$$\mathbf{e}_{\text{SOF}} = \cos\theta_{1,2} \{-\sin\varphi, \cos\varphi, 0\}.$$
(45)

One can see that the corresponding SOF has only in-plane components.

For the case (43), we have

$$C_{\text{SOC}} = \frac{2}{3} (\alpha_{WZ} + b\gamma_{WZ} \langle k_z^2 \rangle),$$

$$\mathbf{e}_{\text{2DEG}} = \{-\sin\varphi, \cos\varphi\},$$

$$\mathbf{e}_{\text{SOF}} = \{\cos\theta_{3,4}\cos\varphi, \cos\theta_{3,4}\sin\varphi, \sin\theta_{3,4}\}.$$
(46)

It is easy to check that the vectors \mathbf{e}_{2DEG} and \mathbf{e}_{SOF} are orthogonal for both cases.

For a concrete type of the confinement potential of the WZ QW it is possible to estimate values of the QW width that allow existence of the solutions (42) and (43). To do

this, we use the values of α_{WZ} , γ_{WZ} , and *b* for GaAs, GaSb, InAs, and InSb in the wurtzite phase obtained by Gmitra and Fabian from first-principles calculations with lattice constants values measured in wurtzite nanowires [50]. As it was earlier for ZB QWs, we assume $\langle k_z^2 \rangle = (\pi/d)^2$ corresponding to an infinite quantum square well of width *d* and calculate values of *d*, for which $-2 \le \xi \le 1$. Results of these calculations are presented in Table IV. Their analysis shows that the calculated values of the QW widths are, in principle, achievable for modern nanotechnologies, although we note that a reliable determination of α_{WZ} , γ_{WZ} , and *b* in bulk wurtzite semiconductors is needed for more definite conclusions.

In the above consideration of the WZ 2DES we only take into account the Dresselhaus and the WZ intrinsic Rashba-like contributions, which strengths are determined by the parameters γ_{WZ} and α_{WZ} , respectively. Inclusion of the additional Rashba term (20) with the parameter α_{210} modifies the SOC vectors γ_{10} and γ_{01} , and leads to the following function f_1 :

$$f_1 = (\cos\theta(\Gamma + b - 3\eta(\theta)) - \Gamma_R)^2 [\sin^2\theta(\Gamma + b - \eta(\theta))^2 + (\cos\theta(\Gamma + b - \eta(\theta)) - \Gamma_R)^2],$$
(47)

where $\Gamma_R = \frac{\alpha_{210}}{\gamma_{WZ} \langle k_z^2 \rangle}$.

For [0001] WZ QWs, combination of the relations (20), (38), and (39) yields

$$\hat{H}_{WZ}^{(1)[0001]} + \hat{H}_{R}^{(1)} = \left(\alpha_{WZ} + \gamma_{WZ}b\langle k_{z}^{2} \rangle - \alpha_{210}\right) \left(\hat{\sigma}_{x}\hat{k}_{y} - \hat{\sigma}_{y}\hat{k}_{x}\right).$$
(48)

The functional form of the k-linear SOC Hamiltonian (48) coincides with the form of the Rashba Hamiltonian (20) and the only possibility to satisfy the condition $f_1 = 0$ is to vanish the combination $\alpha_{WZ} + \gamma_{WZ} b \langle k_z^2 \rangle - \alpha_{210}$. In principle, it can be achieved through manipulation of the parameter α_{210} by means of external electric field (see also [43]).

The other values of the angle θ , for which the SOF is collinear in the presence of the Rashba term (20) can be obtained from the cubic in $\cos \theta$ equation

$$3\cos^{3}\theta - (\xi + 2)\cos\theta - \Gamma_{R}/(b+1) = 0.$$
(49)

Depending on the values of the parameters α_{WZ} , γ_{WZ} , *b*, and α_{210} , which determine its coefficients, it can have different number of real roots.

VI. SUMMARY

In this paper, we have theoretically studied 2D electron systems that are described by the effective Hamiltonians containing SOC terms up to (2n + 1)-th order in wave vector **k**. The general condition for realizing a collinear SOF in such systems formulated only in terms of the SOC parameters has been derived. We have computed the complete set of the **k**-cubic Dresselhaus SOC contributions to the effective 2D spin Hamiltonian of an arbitrarily oriented ZB QW by averaging along the growth direction of the bulk Dresselhaus Hamiltonian of fifth order in **k** within the lowest conduction subband. Together with accounting of the known expressions for the **k**-cubic Rashba terms in ZB QWs of certain orientations it leads to some interesting results.

For asymmetric [001] ZB QWs, we find two combinations of the SOC parameters yielding the collinear SOF even in the presence of the **k**-cubic SOC terms. Next, we explicitly prove within our formalism that the SOF is collinear at all orders in **k** in [110] symmetric ZB QWs (see the Appendix). According to our calculations, there also remain some possibilities for realization of the collinear SOF in [111] and [113] ZB QWs, although restrictions imposed on the SOC parameters in these two cases are strong enough. In [013] ZB QWs, the collinear SOF cannot be realized even in the presence of only the **k**linear Dresselhaus and Rashba SOC contributions.

We have also considered wurtzite-type 2D systems, which are characterized by the effective Hamiltonians containing only **k**-linear SOC terms. Our analysis reveals existence of some peculiar orientations of the 2DEG plane, for which the corresponding SOF is collinear. These findings can be used as the basis for future research of the persistent spin helices in the wurtzite-type semiconductor 2DEG.

In this paper, we do not take into account effects of the interface inversion asymmetry [36,37,51–54] and strain [47,55], which may give significant contributions to SOC in QWs with a peculiar design (growth direction, width, and the other details). Both reliable experimental determination of the SOC vectors and extraction of the SOC parameters with usage of the more complicated computational approaches are needed for verification of the presented results.

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APPENDIX: COLLINEARITY OF THE SPIN-ORBIT EFFECTIVE MAGNETIC FIELD IN SYMMETRIC [110] ZINC-BLENDE OWS

It is implied from the symmetry considerations that in symmetric [110] ZB QWs the electron spin is perpendicular to the QW plane [29]. In this Appendix, we demonstrate within the present formalism that the SOF is collinear at all orders in wave vector \mathbf{k} in such QWs.

We rotate the Hamiltonian (15) such that the *z* axis of the transformed system is aligned with the [110] direction. The operators $\hat{\mathbf{k}}_1$ and $\hat{\sigma}_1$ in the initial coordinate system are connected with the operators $\hat{\mathbf{k}}$ and $\hat{\sigma}$ in the transformed system as $\hat{\mathbf{k}}_1 = M\hat{\mathbf{k}}, \hat{\sigma}_1 = M\hat{\sigma}$ via the matrix

$$M = \frac{1}{2} \begin{vmatrix} 1 & -1 & \sqrt{2} \\ -1 & 1 & \sqrt{2} \\ -\sqrt{2} & -\sqrt{2} & 0 \end{vmatrix}.$$
 (A1)

Substitutions $\hat{\mathbf{k}}_1 = M\hat{\mathbf{k}}$ and $\hat{\boldsymbol{\sigma}}_1 = M\hat{\boldsymbol{\sigma}}$ in Eq. (15) together with standard trigonometric transformations allow us to write the transformed Hamiltonian in the form

$$\begin{aligned} \hat{H}_{\text{bulk}} &= E_0(f(\hat{k}_x, \hat{k}_y, \hat{k}_z)(\hat{\sigma}_x + \hat{\sigma}_y) \\ &+ f^{(-)}(\hat{k}_x, \hat{k}_y, \hat{k}_z)(\hat{\sigma}_x - \hat{\sigma}_y) \\ &+ \sqrt{2} f^{(+)}(\hat{k}_x, \hat{k}_y, \hat{k}_z)\hat{\sigma}_z), \end{aligned}$$
(A2)

with functions

$$f(\hat{k}_{x}, \hat{k}_{y}, \hat{k}_{z}) = \sqrt{2} \sin\left(\frac{a}{4}(-\hat{k}_{x} + \hat{k}_{y})\right)$$

$$\times \sin\left(\frac{\sqrt{2}a}{4}(\hat{k}_{x} + \hat{k}_{y})\right) \sin\left(\frac{\sqrt{2}a}{4}\hat{k}_{z}\right),$$

$$f^{(\pm)}(\hat{k}_{x}, \hat{k}_{y}, \hat{k}_{z}) \equiv f^{(\pm)}(\hat{k}_{+}, \hat{k}_{-}, C\hat{k}_{z})$$

$$= \sin(\hat{k}_{+} - C\hat{k}_{z})\sin(\hat{k}_{-} + C\hat{k}_{z})$$

$$\times \sin(\hat{k}_{+} - \hat{k}_{-} + 2C\hat{k}_{z})$$

$$\pm \sin(\hat{k}_{+} + C\hat{k}_{z})\sin(\hat{k}_{-} - C\hat{k}_{z})$$

where

$$\hat{k}_{\pm} = a((\sqrt{2} \pm 1)\hat{k}_x + (\sqrt{2} \mp 1)\hat{k}_y)/8$$
 and $C = \sqrt{2}a/8$.

 $\times \sin(\hat{k}_{+} - \hat{k}_{-} - 2C\hat{k}_{\tau}),$

(A3)

It is easy to see that the functions f and $f^{(-)}$ are odd in \hat{k}_z , while the function $f^{(+)}$ is even, i.e.,

$$f(\hat{k}_x, \hat{k}_y, -\hat{k}_z) = -f(\hat{k}_x, \hat{k}_y, \hat{k}_z),$$

$$f^{(-)}(\hat{k}_x, \hat{k}_y, -\hat{k}_z) = -f^{(-)}(\hat{k}_x, \hat{k}_y, \hat{k}_z)$$

and

$$f^{(+)}(\hat{k}_x, \hat{k}_y, -\hat{k}_z) = f^{(+)}(\hat{k}_x, \hat{k}_y, \hat{k}_z).$$

The latter means that after averaging of the Hamiltonian (A2) along the growth direction (the *z* axis) within the lowest subband, we obtain an effective 2D SOC Hamiltonian, which contains only terms proportional to $\hat{\sigma}_z$. The **k**-linear, **k**-cubic or the effective 2D Hamiltonians of a higher order in **k**, which can be derived by expansion of this Hamiltonian about the Γ point, also contain terms with $\hat{\sigma}_z$ only. In other words, the corresponding SOF is collinear to [110] direction at all orders in wave vector **k** in symmetric [110] ZB QWs.

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