Persistent spin helices in 2D electron systems

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Abstract. We present a theoretical investigation of persistent spin helices in two-dimensional electron systems with spin-orbit coupling. For this purpose, we consider a single-particle effective mass Hamiltonian with a generalized linear-in-***k*** spin-orbit coupling term corresponding to a quantum well grown in an arbitrary crystallographic direction, and derive the general condition for the formation of the persistent spin helix. This condition applied for the Hamiltonians describing quantum wells with different growth directions indicates the possibility of existence of the persistent spin helix in a wide class of 2D systems apart from the [001] model with equal Rashba and Dresselhaus spin-orbit coupling strengths and the [110] Dresselhaus model.

1. Introduction

Although properties of two-dimensional electron gas (2DEG) with spin-orbit coupling (SOC) have been studied intensively during several decades [1], some of its fascinating features were established relatively recently. In 2006 Bernevig et al. [2] discovered a new type of SU(2) spin rotation symmetry for two well-known special cases of 2DEG with SOC: the [001] model with equal Rashba and Dresselhaus SOC strengths (ReD model) and the Dresselhaus [110] model. They predicted the persistent spin helix (PSH) which is a special spin precession pattern with the precession angle depending only on the net displacement in specific directions (±[110] for the ReD model and ±[1 $\bar{1}$ 0] for the Dresselhaus [110] model). In 2009, PSHs were experimentally observed in [001]-grown GaAs/AlGaAs quantum wells (QWs) [3] and since then many theoretical [4-8] and experimental [9-15] investigations have been devoted to the studies of different manifestations of the PSH. However, almost all of them primarily focus on two above-mentioned cases and do not cover the other types of 2D electron systems with SOC. The main goal of the present paper is to derive the general condition of the PSH formation in 2DEG contained in a QW grown in an arbitrary crystallographic direction and outline some specific materials that are good candidates for realization of the PSH state.

2. The generalized SOC-Hamiltonian

Motivated by our main goal, we consider the following generalized form of a single-particle effective mass Hamiltonian with linear-in-***k*** SOC:

$$\hat{H} = \frac{\hbar^2}{2m}\left(\hat{k}_x^2 + \hat{k}_y^2\right)\hat{\sigma}_0 + \left(\alpha_{11}\hat{\sigma}_x + \alpha_{12}\hat{\sigma}_y + \alpha_{13}\hat{\sigma}_z\right)\hat{k}_x + \left(\alpha_{21}\hat{\sigma}_x + \alpha_{22}\hat{\sigma}_y + \alpha_{23}\hat{\sigma}_z\right)\hat{k}_y , \qquad (1)$$

where we use Cartesian coordinates with z axis perpendicular to the plane of 2DEG, m is the effective electron mass, six parameters α_{ij} define the asymmetry induced SOC, $\hat{\sigma}_0$ and $\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$ are the 2×2 unit matrix and the Pauli matrices, respectively.

In [6, 16] it was shown that the Rashba and Dresselhaus SOC in two dimensions can be regarded as a Yang-Mills non-Abelian gauge field. Following the approach developed in [6], we introduce the SOC gauge

$$\hat{\vec{\gamma}}^{SO} = \{\hat{\gamma}_x, \hat{\gamma}_y\} = \frac{m}{\hbar}\left\{\left(\vec{\alpha}_1 \cdot \hat{\vec{\sigma}}\right), \left(\vec{\alpha}_2 \cdot \hat{\vec{\sigma}}\right)\right\}, \tag{2}$$

and rewrite the Hamiltonian (1) in the form:

$$\hat{H} = \frac{1}{2m}\left(\left(\hat{p}_x\hat{\sigma}_0 + \hat{\gamma}_x\right)^2 + \left(\hat{p}_y\hat{\sigma}_0 + \hat{\gamma}_y\right)^2\right) - V\hat{\sigma}_0, \tag{3}$$

with the constant potential $V = \left(|\vec{\alpha}_1|^2 + |\vec{\alpha}_2|^2\right)/2\hbar^2$, where $\vec{\alpha}_1 = \{\alpha_{11}, \alpha_{12}, \alpha_{13}\}$ and $\vec{\alpha}_2 = \{\alpha_{21}, \alpha_{22}, \alpha_{23}\}$ are two symbolic vectors constructed from the SOC parameters. In general, the components of the SO gauge do not commute,

$$\left[\hat{\gamma}_x, \hat{\gamma}_y\right] = \mathrm{i}\frac{2m^2}{\hbar^2}\left(\hat{\vec{\sigma}} \cdot [\vec{\alpha}_1 \times \vec{\alpha}_2]\right). \tag{4}$$

However, if the cross product of $\vec{\alpha}_1$ and $\vec{\alpha}_2$ is a null vector, the commutator (4) vanishes. In such situations, the operator of the spin projection on the direction $\vec{\alpha}_1$ commutes with the Hamiltonian (1) and defines an extra conserved physical quantity. Moreover, in these exceptional symmetric cases, the effective SOC-induced magnetic field with components $\left\{\alpha_{11}\hat{k}_x + \alpha_{21}\hat{k}_y,\ \alpha_{12}\hat{k}_x + \alpha_{22}\hat{k}_y,\ \alpha_{13}\hat{k}_x + \alpha_{23}\hat{k}_y\right\}$ becomes unidirectional, i.e. its direction does not depend on the components of the wave vector and is defined by the unit vector $\vec{b} = \vec{\alpha}_2/|\vec{\alpha}_2|$, and the Hamiltonian (1) can be written in the form as $\hat{H}_{SO} = \left(q\hat{k}_x + \hat{k}_y\right)\left(\vec{\alpha}_2 \cdot \hat{\vec{\sigma}}\right)$, where a real constant q is determined from the relation $\vec{\alpha}_1 = q\vec{\alpha}_2$.

Performing the global spin rotation generated by the operator

$$\hat{U} = \hat{\sigma}_0 \cos\frac{\chi}{2} - \mathrm{i}\left(n_x\hat{\sigma}_x + n_y\hat{\sigma}_y\right)\sin\frac{\chi}{2}, \tag{5}$$

where $\vec{n} = \left[\vec{b} \times \vec{e}_z\right] = \left\{\alpha_{22}\big/\sqrt{\alpha_{21}^2 + \alpha_{22}^2},\ -\alpha_{21}\big/\sqrt{\alpha_{21}^2 + \alpha_{22}^2},\ 0\right\}$ with $\vec{e}_z = \{0, 0, 1\}$, and χ is the angle between $\vec{e}_z$ and $\vec{b}$ (see figure 1), we transform the Hamiltonian (1) to the diagonal form:

$$\hat{H}_1 = \frac{\hbar^2}{2m}\left(\hat{k}_x^2 + \hat{k}_y^2\right)\hat{\sigma}_0 + |\vec{\alpha}_2|\left(q\hat{k}_x + \hat{k}_y\right)\hat{\sigma}_z. \tag{6}$$

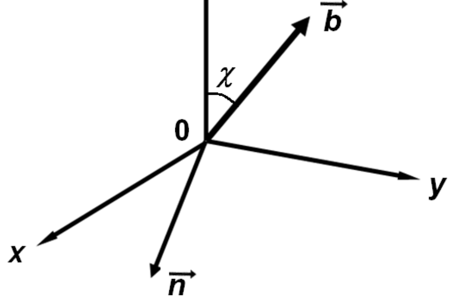

Figure 1. Global transformation generated by the operator (5) is a rotation on the angle χ around the $\vec{n}$ axis which is perpendicular to the direction of the unidirectional effective magnetic field and z axis.

Physically, it means that the direction of the effective magnetic field is chosen as the spin quantization axis and the quantum states are characterized by the projection of the electron spin on this axis.

The energy spectrum of the Hamiltonian (6)

$$E_\lambda(k_x,k_y)=\frac{\hbar^2}{2m}\left(k_x^2+k_y^2\right)+\lambda|\vec{\alpha}_2|\left(qk_x+k_y\right) \tag{7}$$

with $\lambda=\pm1$ which numerates the energy bands, has an important shifting property

$$E_{-1}(k_x+Q_x,k_y+Q_y)=E_1(k_x,k_y) \quad \Leftrightarrow \quad E_{-1}(\vec{k}+\vec{Q})=E_1(\vec{k}), \tag{8}$$

where $\vec{Q}=\frac{2m|\vec{\alpha}_2|}{\hbar^2}\{q,\,1\}$ is the so-called "magic" vector [2]. Accordingly, the eigenfunctions of the Hamiltonian (6) corresponding to quantum numbers $\lambda=\pm1$ have the following simple form:

$$\psi_{\vec{k},1}=\exp\left(\mathrm{i}\left(\vec{k}\cdot\vec{r}\right)\right)\begin{Vmatrix}1\\0\end{Vmatrix}, \qquad \psi_{\vec{k},-1}=\exp\left(\mathrm{i}\left(\vec{k}\cdot\vec{r}\right)\right)\begin{Vmatrix}0\\1\end{Vmatrix}. \tag{9}$$

The ReD and [110] Dresselhaus models being particular cases of the Hamiltonian (6) are characterized by the exact SU(2) symmetry which is introduced in [2] in terms of creation and annihilation operators corresponding to the many-particle problem. Below we demonstrate that the Hamiltonian (6) has the same SU(2) symmetry with generators which are the single-particle counterparts of the generators presented in [2]. Namely, two single-particle operators

$$\begin{aligned}\hat{C}_{\vec{Q}}^{+}&=\frac{\exp\left(-\mathrm{i}\left(\vec{Q}\cdot\vec{r}\right)\right)}{2}\left(\hat{\sigma}_x+\mathrm{i}\hat{\sigma}_y\right)=\exp\left(-\mathrm{i}\left(\vec{Q}\cdot\vec{r}\right)\right)\begin{Vmatrix}0&1\\0&0\end{Vmatrix},\\ \hat{C}_{\vec{Q}}^{-}&=\frac{\exp\left(\mathrm{i}\left(\vec{Q}\cdot\vec{r}\right)\right)}{2}\left(\hat{\sigma}_x-\mathrm{i}\hat{\sigma}_y\right)=\exp\left(\mathrm{i}\left(\vec{Q}\cdot\vec{r}\right)\right)\begin{Vmatrix}0&0\\1&0\end{Vmatrix},\end{aligned} \tag{10}$$

that act on the eigenfunctions (9) in the following way:

$$\hat{C}_{\vec{Q}}^{+}\psi_{\vec{k},-1}=\psi_{\vec{k}-\vec{Q},1}\,,\quad \hat{C}_{\vec{Q}}^{+}\psi_{\vec{k},1}=0\,,\quad \hat{C}_{\vec{Q}}^{-}\psi_{\vec{k},-1}=0\,,\quad \hat{C}_{\vec{Q}}^{-}\psi_{\vec{k},1}=\psi_{\vec{k}+\vec{Q},-1}\,, \tag{11}$$

together with $\hat{\sigma}_z$ obey the commutation relation for the angular momentum operator

$$\left[\hat{\sigma}_z,\hat{C}_{\vec{Q}}^{+}\right]=2\hat{C}_{\vec{Q}}^{+}\,,\quad \left[\hat{\sigma}_z,\hat{C}_{\vec{Q}}^{-}\right]=-2\hat{C}_{\vec{Q}}^{-}\,,\quad \left[\hat{C}_{\vec{Q}}^{+},\hat{C}_{\vec{Q}}^{-}\right]=\hat{\sigma}_z\,. \tag{12}$$

In addition, due to the shifting property (8) $\hat{C}_{\vec{Q}}^{+}$ and $\hat{C}_{\vec{Q}}^{-}$ commute with the Hamiltonian (6):

$$\left[\hat{H}_1,\hat{C}_{\vec{Q}}^{+}\right]=\left(E_1(\vec{k}-\vec{Q})-E_{-1}(\vec{k})\right)\hat{C}_{\vec{Q}}^{+}=\hat{0}\,,\qquad \left[\hat{H}_1,\hat{C}_{\vec{Q}}^{-}\right]=\left(E_{-1}(\vec{k}+\vec{Q})-E_1(\vec{k})\right)\hat{C}_{\vec{Q}}^{-}=\hat{0}\,. \tag{13}$$

It is also obvious that $\left[\hat{H}_1,\hat{\sigma}_z\right]=\hat{0}$. The latter relation together with (13) show that single-particles operators $\hat{C}_{\vec{Q}}^{+}$, $\hat{C}_{\vec{Q}}^{-}$ and $\hat{\sigma}_z$ are generators of the exact SU(2) symmetry responsible for formation of the PSH state. Concrete examples of 2D electron systems, where the PSH patterns are expected to appear, are given in the next section.

3. What 2D electron structures are good candidates for realization of the PSH state?

The obtained condition $\left[\vec{\alpha}_1\times\vec{\alpha}_2\right]=\vec{0}$, in fact, defines the possibility of formation of the PSH patterns in arbitrary 2D electron systems with SOC. Nevertheless, the most attractive structures for experimental realization of the PSH state are expected to be found in specific QWs due to opportunities of the SOC parameters manipulation via (a) external electric field and (b) fitting of QW characteristics (type of material and geometrical parameters) for achieving the above-mentioned relation. In this section, we examine a wide class of semiconductor QWs and outline among them some good candidates for realization of the PSH patterns. In addition, relations between the SOC parameters that should be satisfied in order to achieve the PSH state will be obtained.

We begin the analysis with the zinc-blende type QWs. In such structures, the absence of inversion symmetry in the bulk material leads to the Dresselhaus SOC-Hamiltonian:

$$\hat{H}_D = \beta_{ij}\,\hat{k}_i\,\hat{\sigma}_j\,, \tag{14}$$

with six parameters β_{ij} ($i = x, y, j = x, y, z$). Exact expression of the Dresselhaus term depends on the QW growth direction. The other contribution to the SOC-Hamiltonian is connected with the structure inversion asymmetry and described by the Rashba term:

$$\hat{H}_R = \alpha_R\left(\hat{k}_x\hat{\sigma}_y - \hat{k}_y\hat{\sigma}_x\right). \tag{15}$$

Hereafter, we divide all zinc-blende QWs into symmetric (the corresponding Hamiltonian contains only the Dresselhaus term) and asymmetric (both Dresselhaus and Rashba terms are present) types. SOC-parts of the electron effective mass Hamiltonians corresponding to different QWs are presented in table 1. Application of the criterion $[\vec{\alpha}_1\times\vec{\alpha}_2]=\vec{0}$ for every Hamiltonian from this table allows to conclude whether the PSH state is realized in a specific QW or not.

Table 1. Formation of the PSH in symmetric (S) and asymmetric (A) QWs with different growth direction. All SOC Hamiltonians are taken from [17] and correspond to materials with zinc-blende structure.

Growth direction	SOC-Hamiltonian	$\vec{\alpha}_1$ and $\vec{\alpha}_2$	Existence of the PSH	Relation between the SOC parameters when the PSH state is realized
[001]	S: $\hat{H} = \beta\left(\hat{k}_x\hat{\sigma}_x - \hat{k}_y\hat{\sigma}_y\right)$	$\vec{\alpha}_1 = \{\beta,0,0\}$, $\vec{\alpha}_2 = \{0,-\beta,0\}$	No	–
	A: $\hat{H} = \beta\left(\hat{k}_x\hat{\sigma}_x - \hat{k}_y\hat{\sigma}_y\right) + \alpha\left(\hat{k}_y\hat{\sigma}_x - \hat{k}_x\hat{\sigma}_y\right)$	$\vec{\alpha}_1 = \{\beta,-\alpha,0\}$, $\vec{\alpha}_2 = \{\alpha,-\beta,0\}$	Yes	$\lvert\alpha\rvert = \lvert\beta\rvert$
[110]	S: $\hat{H} = \beta\,\hat{k}_x\hat{\sigma}_z$	$\vec{\alpha}_1 = \{0,0,\beta\}$, $\vec{\alpha}_2 = \{0,0,0\}$	Yes	$\beta \neq 0$
	A: $\hat{H} = (\beta_1+\alpha)\hat{k}_y\hat{\sigma}_x + (\beta_2-\alpha)\hat{k}_x\hat{\sigma}_y + \beta_3\,\hat{k}_x\hat{\sigma}_z$	$\vec{\alpha}_1 = \{0,\beta_2-\alpha,\beta_3\}$, $\vec{\alpha}_2 = \{\beta_1+\alpha,0,0\}$	Yes	$\beta_1+\alpha=0$ or $(\beta_2-\alpha)^2+\beta_3^2=0$
[111]	S: $\hat{H} = \beta\left(\hat{k}_y\hat{\sigma}_x - \hat{k}_x\hat{\sigma}_y\right)$	$\vec{\alpha}_1 = \{0,-\beta,0\}$, $\vec{\alpha}_2 = \{\beta,0,0\}$	No	–
	A: $\hat{H} = (\alpha+\beta)\left(\hat{k}_y\hat{\sigma}_x - \hat{k}_x\hat{\sigma}_y\right)$	$\vec{\alpha}_1 = \{0,-(\alpha+\beta),0\}$, $\vec{\alpha}_2 = \{\alpha+\beta,0,0\}$	No	–
[113]	S: $\hat{H} = \beta_1\hat{k}_y\hat{\sigma}_x + \beta_2\hat{k}_x\hat{\sigma}_y + \beta_3\hat{k}_x\hat{\sigma}_z$	$\vec{\alpha}_1 = \{0,\beta_2,\beta_3\}$ $\vec{\alpha}_2 = \{\beta_1,0,0\}$	Yes	$\beta_1=0$ or $\beta_2=\beta_3=0$
	A: $\hat{H} = (\beta_1+\alpha)\hat{k}_y\hat{\sigma}_x + (\beta_2-\alpha)\hat{k}_x\hat{\sigma}_y + \beta_3\hat{k}_x\hat{\sigma}_z$	$\vec{\alpha}_1 = \{0,\beta_2-\alpha,\beta_3\}$, $\vec{\alpha}_2 = \{\beta_1+\alpha,0,0\}$	Yes	$\beta_1+\alpha=0$ or $(\beta_2-\alpha)^2+\beta_3^2=0$

Firstly, in the most studied case of [001] QWs, the helices are not formed when a well is symmetric and appear in asymmetric wells only if modules of the Rashba and Dresselhaus SOC strengths are equal (ReD model). This result agrees with previous investigations [2-4, 6, 11-14]. Secondly, the PSH structures exist in the symmetric [110] QW for any value of the Dresselhaus SOC strength. This case is known as the Dresselhaus [110] model. In order to guarantee the formation of the PSH it is necessary just to prepare a symmetric well. Therefore, such kind of QWs seems very attractive for realization of the PSH state.

Application of the general condition allows to find all possible 2D systems apart from the ReD and Dresselhaus [110] models which provide the formation of the PSHs. In particular, our calculations show that the PSH patterns can also be realized for some combinations of the SOC parameters in [110]-asymmetric and [113] QWs. Apparently, they are expected to appear in [112] and miscut [001] QWs.

For QWs prepared on [013]-oriented substrates belonging to the trivial point group C_1, there are no restrictions on the relation between the spin and wavevector components arising from the symmetry requirements. Hence, the SOC-Hamiltonian for such systems has the most general form and coincides with the spin-orbit part of the Hamiltonian (1). We pay attention to this case because of the fact that [013]-oriented substrates are used for growth of HgTe-based 2D topological insulators [17].

In our analysis we neglected the interface inversion asymmetry which may yields extra linear-in-$\boldsymbol{k}$ terms in the Hamiltonian (1) caused by noninversion symmetric bonding of atoms at a heterostructure interface [18-20]. Although such contributions in the SOC have the same form as the Dresselhaus term in [001] QWs made from III-V materials, their inclusion may be important for formation of the PSH state in [110] QWs [21] and essential for SiGe QWs [22]. Therefore, effects of the interface inversion asymmetry should be taken into account in more rigorous investigations in the above-mentioned systems.

In summary of this section, our analysis points on the possibility of the PSH patterns formation in a wide class of 2D electron systems. In a specific QW, the PSH regime can be achieved through manipulation of the Rashba SOC be means of external electric field or (and) adjustment of the Dresselhaus SOC parameters by fitting of the QW width and other details of its design.

4. Conclusion
In conclusion, we have theoretically studied the spin precession in 2D electron systems with SOC and have derived the general condition of the PSH state realization. This condition applied for the Hamiltonians describing QWs with different growth directions indicates the possibility of existence of the PSH patterns in a wide class of 2D systems including the well-studied [001] model with equal the Rashba and Dresselhaus SOC strengths and the [110] Dresselhaus model. The latter statement requires experimental verification and we hope that the appropriate studies will be realized soon.

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