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FAST TRACK COMMUNICATION

The surface Rashba effect: a $\boldsymbol{k}\cdot\boldsymbol{p}$ perturbation approach

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Abstract

For surface systems, the Rashba effect is studied by using a $k\cdot p$ perturbation method. It is shown that the velocity-operator term in the perturbation gives the generalized Rashba Hamiltonian, of which a group-theoretical analysis is given to explain variations in the spin splitting and spin structure expected for typical surface symmetry. The matrix elements of the velocity and spin-angular-momentum operators play a key role in determining the characteristic features of the surface Rashba effect. Whether a surface system shows isotropic spin splitting and vortical spin structure as given by the original Rashba Hamiltonian or not depends on the group of k appearing in the corresponding two-dimensional Brillouin zone. It is especially emphasized that the ideal Rashba effect may be realized even for a wavevector $\boldsymbol{k}$ without time reversal, which is usually believed to be a necessary condition.

1. Introduction

Recently, much attention has been drawn to phenomena originating from spin–orbit coupling (SOC), such as the magnetoelectric effect [1], spin Hall effect [2], Rashba effect [3], and so on. Among these, the Rashba effect has been recently observed in a variety of surface systems by means of angle-resolved photoemission spectroscopy measurements [4–14]. Originally, the Rashba effect was studied as a phenomenon of spin splitting by an applied electric field in two-dimensional (2D) electron gas systems [15]. The Rashba Hamiltonian originating from SOC is given as

$$\mathcal{H}_{\mathrm{R}} = \alpha_{\mathrm{R}} \left(\hat{z} \times \hbar \boldsymbol{k}\right) \cdot \boldsymbol{s} \tag{1}$$

for a free electron with momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$ and spin $\boldsymbol{s}$ under an electric field $\boldsymbol{E} = \mathcal{E}\hat{z}$. Similar spin splitting can be generally seen for bulk systems with large SOC and broken inversion symmetry [16]. The characteristic features of the Rashba Hamiltonian in equation (1) are the isotropic spin splitting linear in k and the vortical spin structure, around the center of the Brillouin zone (BZ).

The surface Rashba effect has been extensively investigated by means of band-theoretical calculations with SOC included [17–22]. A simple tight-binding model with SOC has been used to study the spin splitting for a surface state on Au(111) and it is found that the splitting depends on the magnitude of the SOC and the surface potential [17]. First-principles calculations [18–22] have been performed for Bi(111), Gd(0001), Ag(111), Au(111), Lu(0001) and Sb(111) surfaces and Ag(111)–Bi, Ag(111)–Pb and Si(111)–Bi adsorbed surfaces, and these have shown that SOC is crucial in the close vicinity of the nucleus and the Rashba spin splitting originates from the asymmetry of the surface-state electron density about the nucleus rather than the surface potential.

It is widely believed that Rashba spin splitting may happen around $\boldsymbol{k}$ points that have time reversal. This leads to the Rashba effect possibly appearing around BZ boundary points in addition to the BZ center [22]. Figure 1 shows $\boldsymbol{k}$ points with time reversal in the 2D BZ of square, rectangular and triangular lattices. Note that $\bar{\mathrm{K}}$ in the triangular BZ has no time reversal. However, it has been shown for the Si(111)–Bi system [22] that ideal Rashba spin splitting and spin vorticity around $\bar{\mathrm{K}}$ points are actually predicted. Furthermore, the spin structure of Rashba-split bands around $\bar{\mathrm{M}}$ that has time reversal is not vortical, but hyperbolic. Although some symmetry arguments have been given for the spin splitting and spin structure, under

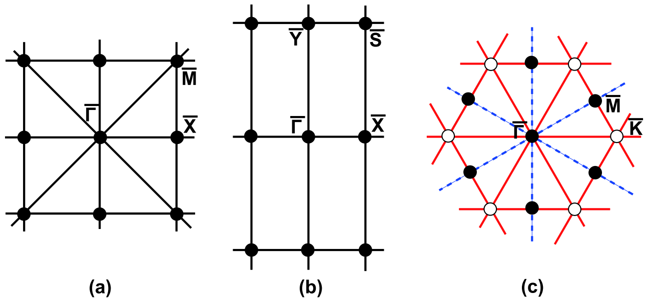

Figure 1. Two-dimensional Brillouin zone (BZ) of (a) square lattice (plane group $p4mm$), (b) rectangular lattice ($p2mm$) and (c) triangular lattice ($p3m1$ and $p31m$). Solid dots denote $\boldsymbol{k}$ points which have time-reversal symmetry. Note that $\bar{\mathrm{K}}$ represented by an open circle in the triangular BZ has no time reversal. Solid black lines represent $\boldsymbol{k}$ points which have mirror symmetry in (a) and (b). In (c), blue broken (red solid) lines indicate $\boldsymbol{k}$ points which have mirror symmetry for the plane group $p3m1$ ($p31m$).

(This figure is in colour only in the electronic version)

which conditions the isotropic spin splitting and spin vorticity as given by the Rashba Hamiltonian in equation (1) appear are still unclear.

In this paper, the spin splitting and spin structure brought about by SOC in surface systems are generally studied on the basis of a $k \cdot p$ perturbation theory. It is pointed out that the velocity-operator term in the perturbation leads to the generalized Rashba Hamiltonian. The matrix elements of the velocity and spin-angular-momentum operators which are key in the Rashba effect are inspected via group-theoretical consideration. Conditions for the ideal Rashba effect and some variations in the spin splitting and spin structure are examined for the relevant irreducible representations belonging to the groups of k in typical 2D BZ.

2. $\boldsymbol{k} \cdot \boldsymbol{p}$ perturbation theory

A Pauli-type (Schrödinger + SOC) one-electron Hamiltonian is given in Ryd atomic units as

$$\mathcal{H} = \boldsymbol{p}^2 + V + c^{-2} (\nabla V \times \boldsymbol{p}) \cdot \boldsymbol{\sigma}$$

where V is the crystal potential, c is the velocity of light, and $\boldsymbol{s}$ is represented with the Pauli matrix $\boldsymbol{\sigma}$ as $\boldsymbol{s} = \boldsymbol{\sigma}/2$. With the knowledge of eigenstates at a wavevector $\boldsymbol{k}$

$$\mathcal{H}\psi(\boldsymbol{k}, \boldsymbol{r}) = E(\boldsymbol{k})\psi(\boldsymbol{k}, \boldsymbol{r})$$

we solve the equation for $\boldsymbol{k} + \boldsymbol{q}$ with

$$\psi(\boldsymbol{k} + \boldsymbol{q}, \boldsymbol{r}) = \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \chi(\boldsymbol{k}, \boldsymbol{r})$$

and the one-electron equation becomes

$$H(\boldsymbol{q})\chi(\boldsymbol{k}, \boldsymbol{r}) = E(\boldsymbol{k} + \boldsymbol{q})\chi(\boldsymbol{k}, \boldsymbol{r}).$$

Here, the Hamiltonian $H(\boldsymbol{q})$ is given as [23]

$$H(\boldsymbol{q}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \mathcal{H} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} = \mathcal{H} + \boldsymbol{q} \cdot \boldsymbol{v} + \boldsymbol{q}^2. \tag{2}$$

The velocity operator $\boldsymbol{v}$ is expressed as

$$\boldsymbol{v} = 2\boldsymbol{p} + c^{-2} \boldsymbol{\sigma} \times \nabla V \tag{3}$$

and the resulting matrix elements of the Hamiltonian $H(\boldsymbol{q})$ are constructed and solved as

$$H_{mn}(\boldsymbol{q}) = \left[E_m(\boldsymbol{k}) + \boldsymbol{q}^2\right] \delta_{mn} + \boldsymbol{q} \cdot \boldsymbol{v}_{mn}$$

$$E_m(\boldsymbol{k}) = \langle \psi_m(\boldsymbol{k}) | \mathcal{H} | \psi_m(\boldsymbol{k}) \rangle$$

$$\boldsymbol{v}_{mn} = \langle \psi_m(\boldsymbol{k}) | \boldsymbol{v} | \psi_n(\boldsymbol{k}) \rangle.$$

In equation (2), the first-order term in $\boldsymbol{q}$ comes from the velocity operator. Thus, in order to investigate the band structure around $\boldsymbol{k}$, one considers the perturbation of the first order in $\boldsymbol{q}$ given as

$$\begin{aligned} H'(\boldsymbol{q}) &= \boldsymbol{q} \cdot \boldsymbol{v} \\ &= 2\boldsymbol{q} \cdot \boldsymbol{p} + c^{-2} \boldsymbol{q} \cdot \boldsymbol{\sigma} \times \nabla V \end{aligned} \tag{4}$$

which may be regarded as the generalized Rashba Hamiltonian.

3. Matrix elements of velocity and spin-angular-momentum operators

Let us consider how to evaluate the matrix elements of a vector operator $\boldsymbol{a}$ with respect to d degenerate states belonging to an irreducible representation of the group of k. On assuming a symmetry operation R and unperturbed degenerate states $\{\psi_i\}$ ($i = 1, \ldots, d$), the matrix elements are

$$\begin{aligned} \langle \boldsymbol{a} \rangle_{ij} &= \langle \psi_i | \boldsymbol{a} | \psi_j \rangle \\ &= \langle R\psi_i | R\boldsymbol{a}R^{-1} | R\psi_j \rangle \\ &= \sum_{kk'} D^*_{ki}(R) \langle \psi_k | R\boldsymbol{a}R^{-1} | \psi_{k'} \rangle D_{k'j}(R) \\ &= \sum_{kk'} D^*_{ki}(R) \langle R\boldsymbol{a}R^{-1} \rangle_{kk'} D_{k'j}(R) \end{aligned} \tag{5}$$

where $\mathbf{D}(R)$ is the $d \times d$ representation matrix of the irreducible representation for R. The transformation of the operator $\boldsymbol{a}$ in a row vector form can be given as

$$R\boldsymbol{a}R^{-1} = \boldsymbol{a}\mathbf{R}. \tag{6}$$

If $\boldsymbol{a}$ is a polar vector operator such as velocity or momentum, $\mathbf{R}$ is just the 3×3 transformation matrix of the operation R. For an axial vector operator such as the spin angular momentum, on the other hand, $\mathbf{R}$ takes only the proper rotational part because inversion, if included, makes the axial vector invariant. From equations (5) and (6) with replacement $R \to R^{-1}$ and $\mathbf{D}(R^{-1}) = \mathbf{D}^{-1}(R) = \mathbf{D}^\dagger(R)$, one ends up with

$$\langle \boldsymbol{a} \rangle_{ij} \mathbf{R} = \sum_{kk'} D_{ik}(R) D^*_{jk'}(R) \langle \boldsymbol{a} \rangle_{kk'} \tag{7}$$

which is the master equation for the matrix elements in the following discussion. Before applying equation (7) to some particular symmetry cases, general restrictions imposed on the matrix elements are investigated below.

Table 1. Symmetry requirements of the matrix elements of polar and axial vector operators for d-dimensional irreducible representations of the groups of k appearing in the typical two-dimensional Brillouin zone. In C_{1h}, the mirror plane is taken on yz.

Group	d	Polar	Axial
C_2, C_3, C_4	1	$\langle v_x\rangle = \langle v_y\rangle = 0$	$\langle \sigma_x\rangle = \langle \sigma_y\rangle = 0$
		$\langle v_z\rangle \neq 0$	$\langle \sigma_z\rangle \neq 0$
C_{2v}, C_{3v}, C_{4v}	1	$\langle v_x\rangle = \langle v_y\rangle = 0$	$\langle \sigma_x\rangle = \langle \sigma_y\rangle = \langle \sigma_z\rangle = 0$
		$\langle v_z\rangle \neq 0$	
	2	$\langle v_x\rangle_{11} = -\langle v_x\rangle_{22}$	$\langle \sigma_x\rangle_{11} = -\langle \sigma_x\rangle_{22}$
		$\langle v_y\rangle_{11} = -\langle v_y\rangle_{22}$	$\langle \sigma_y\rangle_{11} = -\langle \sigma_y\rangle_{22}$
		$\langle v_z\rangle_{11} = \langle v_z\rangle_{22}$	$\langle \sigma_z\rangle_{11} = -\langle \sigma_z\rangle_{22}$
C_{1h}	1	$\langle v_x\rangle = 0$	$\langle \sigma_x\rangle \neq 0$
		$\langle v_y\rangle \neq 0$	$\langle \sigma_y\rangle = \langle \sigma_z\rangle = 0$
		$\langle v_z\rangle \neq 0$	

Summing equation (7) over all operations in the group of k and by using the orthogonality theorem for the representation matrix, the diagonal matrix elements have a relation

$$\langle \boldsymbol{a}\rangle_{ii} \sum_R \mathbf{R} = \frac{g}{d} \sum_k \langle \boldsymbol{a}\rangle_{kk} \tag{8}$$

where g is the order of the group. When the group contains only proper rotations like C_2, C_3 and C_4, the relation can be reduced to

$$(0, 0, \langle a_z\rangle_{ii}) = \frac{1}{d} \sum_k \langle \boldsymbol{a}\rangle_{kk}$$

for both polar and axial vector operators. This means that the traces of the x and y components are zero and the diagonal elements of the z component are the same as each other. In particular, for C_2, C_3 and C_4, as only one-dimensional representations are involved, the matrix elements of the x and y components are zero and its z counterpart may be non-zero. When the group includes rotational and mirror operations like C_{2v}, C_{3v} and C_{4v}, the same arguments as above can be made for a polar vector operator while the trace of all the components for an axial vector operator becomes zero because of $\sum_R \mathbf{R} = 0$. In the case of the group C_{1h} with one mirror operation, only the mirror-plane components of a polar vector operator and the mirror-normal component of an axial vector operator survive. In figure 1, $\boldsymbol{k}$ lines that have one mirror operation are drawn for 2D BZ. It should be noted that the $\boldsymbol{k}$ lines with the mirror differ between the plane groups $p3m1$ and $p31m$ in the triangular BZ.

The general requirements of the matrix elements of polar and axial vector operators are summarized in table 1 for the groups appearing in the typical 2D BZ. The most interesting point in table 1 is that degenerate states belonging to the 2D irreducible representations in C_{2v}, C_{3v} and C_{4v} can behave just like a time-reversal pair as regards the x and y components of any polar vector operator and all the components of any axial vector operator. This may be why the Rashba effect can take place even for $\boldsymbol{k}$ points that have no time reversal. Among the typical 2D BZ shown in figure 1, only $\bar{K}$ points in the $p31m$ triangular system meet the situation.

Table 2. The group of k at the zone center and some zone boundary points in a typical two-dimensional Brillouin zone.

Lattice (plane group)	k	The group of k
Square ($p4mm$)	$\bar{\Gamma}$, $\bar{M}$	C_{4v}
	$\bar{X}$	C_{2v}
Rectangular ($p2mm$)	$\bar{\Gamma}$, $\bar{X}$, $\bar{M}$	C_{2v}
Triangular ($p3m1$)	$\bar{\Gamma}$	C_{3v}
	$\bar{K}$	C_3
	$\bar{M}$	C_{1h}
Triangular ($p31m$)	$\bar{\Gamma}$, $\bar{K}$	C_{3v}
	$\bar{M}$	C_{1h}

4. Rashba spin splitting and spin structure

If bands show Rashba spin splitting around $\boldsymbol{k}$, they should be degenerate states at $\boldsymbol{k}$ with SOC. The groups of k that have 2D representations in the typical 2D BZ shown in figure 1 are C_{2v}, C_{3v} and C_{4v} as listed in table 2. In addition, 1D representation states in some groups are degenerate by time reversal, for example in C_{1h} at $\bar{M}$ points in the triangular BZ. In this section, the generalized Rashba Hamiltonian in equation (4) is analyzed in detail for such degenerate states by using the master equation for the matrix elements in equation (7).

4.1. C_{3v}: a 2D representation Γ_6

We shall first consider a 2D representation Γ_6 [24] (Γ_4 in Bradley's [25] and Lax's [23] notations) in the group C_{3v}. If one chooses $R = C_3$ among the operations, the transformation matrix is

$$\mathbf{R} = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

for both polar and axial vector operators and the representation matrix is

$$\mathbf{D} = \begin{pmatrix} w^* & 0 \\ 0 & w \end{pmatrix}$$

with $w = e^{\pi i/3}$ [24]. The diagonal matrix element $\{ij\} = \{11\}$ in equation (7) can be written as

$$\langle \boldsymbol{a}\rangle_{11}\mathbf{R} = |w|^2 \langle \boldsymbol{a}\rangle_{11}$$

and its x and y components become zero and so does the $\{22\}$ element (see table 1). As for the off-diagonal $\{12\}$ element,

$$\langle \boldsymbol{a}\rangle_{12}\mathbf{R} = (w^*)^2 \langle \boldsymbol{a}\rangle_{12}$$

and thus, one gets $\langle a_y\rangle_{12} = -i\langle a_x\rangle_{12}$. With the matrix elements for the velocity operator taken as $\langle v_x\rangle_{12} \equiv X$, the perturbation matrix for $\boldsymbol{q} = q(\cos\phi, \sin\phi)$ has the form

$$H'(\boldsymbol{q}) = \begin{pmatrix} 0 & qXe^{-i\phi} \\ qX^*e^{i\phi} & 0 \end{pmatrix} \tag{9}$$

and the perturbation energy is obtained as

$$\varepsilon_\pm = \pm q|X|. \tag{10}$$

This result shows that band splitting linear in q is *isotropic* on the BZ xy plane and proportional to the magnitude of the matrix element of the velocity operator $|X|$. The corresponding eigenstates are

$$|\pm\rangle = \frac{1}{\sqrt{2}}\left(\pm\frac{X}{|X|}\mathrm{e}^{-\mathrm{i}\phi}|1\rangle + |2\rangle\right) \tag{11}$$

with the unperturbed degenerate states $|1\rangle$ and $|2\rangle$. The non-vanishing matrix elements of the spin-angular-momentum operator are $\langle\sigma_x\rangle_{12} = \mathrm{i}\langle\sigma_y\rangle_{12} \equiv \zeta$ and $\langle\sigma_z\rangle_{11} = -\langle\sigma_z\rangle_{22} \equiv Z$ and the expectation values of spin with respect to the eigensolutions are non-vanishing only on xy and become

$$\langle\pm|\sigma_x|\pm\rangle = \pm\frac{1}{|X|}\mathrm{Re}\left(\zeta X^*\mathrm{e}^{\mathrm{i}\phi}\right) \tag{12}$$

$$\langle\pm|\sigma_y|\pm\rangle = \pm\frac{1}{|X|}\mathrm{Im}\left(\zeta X^*\mathrm{e}^{\mathrm{i}\phi}\right) \tag{13}$$

implying that the band-split states are actually a spin reversed pair, and satisfy

$$\boldsymbol{q}\cdot\langle\pm|\boldsymbol{\sigma}|\pm\rangle = 0 \tag{14}$$

$$[\boldsymbol{q}\times\langle\pm|\boldsymbol{\sigma}|\pm\rangle]_z = \mathrm{const} \tag{15}$$

showing *vortical* spin structure.

It is, therefore, concluded that the 2D representation Γ_6 state in $\mathrm{C_{3v}}$ reveals the isotropic spin splitting and vortical spin structure just as given by the Rashba Hamiltonian in equation (1) in any case, regardless of the existence of time reversal. This explains the ideal Rashba effect possibly observed not only around $\bar{\Gamma}$ but also around $\bar{\mathrm{K}}$ with $\mathrm{C_{3v}}$ in the triangular BZ.

4.2. C_{4v}: 2D representations Γ_6 and Γ_7

The next example is given for the group $\mathrm{C_{4v}}$. There are two 2D irreducible representations Γ_6 and Γ_7 in $\mathrm{C_{4v}}$ [23–25]. If one takes $R = \mathrm{C_4}$,

$$\mathbf{R} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the corresponding representation matrix is

$$\mathbf{D} = \begin{pmatrix} \pm u^* & 0 \\ 0 & \pm u \end{pmatrix}$$

with $u = \mathrm{e}^{\pi\mathrm{i}/4}$ and double signs $\pm$ for Γ_6 and Γ_7, respectively [24]. Following the case of $\mathrm{C_{3v}}$, the matrix elements of the perturbation Hamiltonian are inspected and obtained in the same form as for $\mathrm{C_{3v}}$. Thus, the 2D representation states Γ_6 and Γ_7 in $\mathrm{C_{4v}}$ also lead to the ideal Rashba features, isotropic spin splitting and vortical spin structure.

4.3. C_{2v}: a 2D representation Γ_5

A slightly complicated result may be expected for the group $\mathrm{C_{2v}}$. There is one 2D representation Γ_5 in $\mathrm{C_{2v}}$ [23–25]. Taking $R = \mathrm{C_2}$, the transformation matrix is

$$\mathbf{R} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the representation matrix is given as

$$\mathbf{D} = \begin{pmatrix} -\mathrm{i} & 0 \\ 0 & \mathrm{i} \end{pmatrix}$$

for the 2D irreducible representation Γ_5 [24]. For the diagonal matrix element $\{11\}$, one gets

$$\langle\boldsymbol{a}\rangle_{11}\mathbf{R} = \langle\boldsymbol{a}\rangle_{11}$$

and thus the x and y components vanish. The off-diagonal elements are

$$\langle\boldsymbol{a}\rangle_{12}\mathbf{R} = -\langle\boldsymbol{a}\rangle_{12}$$

and the x and y components remain independent. It is, furthermore, found by taking a mirror operation for the matrix elements that the off-diagonal elements of the x and y components are real and pure imaginary, respectively. On assuming $\langle v_x\rangle_{12} \equiv X$ and $\langle v_y\rangle_{12} \equiv -\mathrm{i}Y$ for the non-vanishing off-diagonal matrix elements of the velocity operator, the perturbation matrix for $\boldsymbol{q} = q(\cos\phi, \sin\phi)$ is represented as

$$H'(\boldsymbol{q}) = q\begin{pmatrix} 0 & X\cos\phi - \mathrm{i}Y\sin\phi \\ X\cos\phi + \mathrm{i}Y\sin\phi & 0 \end{pmatrix} \tag{16}$$

and the solutions become

$$\varepsilon_\pm = \pm q|X\cos\phi - \mathrm{i}Y\sin\phi| \tag{17}$$

$$|\pm\rangle = \frac{1}{\sqrt{2}}\left(\pm\frac{X\cos\phi - \mathrm{i}Y\sin\phi}{|X\cos\phi - \mathrm{i}Y\sin\phi|}|1\rangle + |2\rangle\right). \tag{18}$$

It is easily seen that the resulting solutions are reduced to the ones in the cases of $\mathrm{C_{3v}}$ and $\mathrm{C_{4v}}$ if $X = Y$. Thus, when the matrix elements of the velocity operator along the x and y directions in BZ are isotropic, the ideal Rashba effect should be found; otherwise anisotropic spin splitting and/or non-vortical spin structure may possibly happen. Strongly anisotropic spin splitting seen in the Au(110) surface may be caused by a large difference in the matrix elements X and Y due to the anisotropic character of the relevant surface states [14, 22].

4.4. C_{1h}: time-reversal degenerate Γ_3 and Γ_4

As a time-reversal degenerate case, let us consider the band structure around $\bar{\mathrm{M}}$ points in the triangular BZ shown in figure 1. The group of k at $\bar{\mathrm{M}}$ points is $\mathrm{C_{1h}}$ (see table 2), which has two 1D representations Γ_3 and Γ_4 in the double-valued representations [23, 25]. In addition, the $\bar{\mathrm{M}}$ points have time reversal and a time-reversal pair of Γ_3 and Γ_4 states are degenerate and expected to show the Rashba spin splitting.

By assuming the mirror operation Σ with the yz mirror plane for R,

$$\mathbf{R} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

for a polar vector operator and

$$\mathbf{R} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

for an axial vector operator, and the representation matrix for the time-reversal pair states $|3\rangle$ and $|4\rangle$ is

$$\mathbf{D} = \begin{pmatrix} -\mathrm{i} & 0 \\ 0 & \mathrm{i} \end{pmatrix}$$

which can be constructed from the characters in C_{1h} [23]. The diagonal {33} element for a polar vector operator in equation (7) is given as

$$\langle \boldsymbol{a} \rangle_{33} \mathbf{R} = \langle \boldsymbol{a} \rangle_{33}$$

making the x component vanishing. The off-diagonal element is given as

$$\langle \boldsymbol{a} \rangle_{34} \mathbf{R} = -\langle \boldsymbol{a} \rangle_{34}$$

and its y component becomes zero. With use of time reversal, it appears that the non-vanishing matrix elements of the velocity operator are all real and can be set as $\langle v_y \rangle_{33} = -\langle v_y \rangle_{44} \equiv Y$ and $\langle v_x \rangle_{34} = \langle v_x \rangle_{43} \equiv X$ and the perturbation matrix for $\boldsymbol{q} = q(\cos\phi, \sin\phi)$ is then given as

$$H'(\boldsymbol{q}) = q \begin{pmatrix} Y \sin\phi & X\cos\phi \\ X\cos\phi & -Y\sin\phi \end{pmatrix}. \qquad (19)$$

The perturbation energy is then obtained as

$$\varepsilon_{\pm} = \pm q \left(X^2 \cos^2\phi + Y^2 \sin^2\phi \right)^{1/2}. \qquad (20)$$

For $q_x \neq 0$, $q_y = 0$, the solutions can be simply written as

$$\varepsilon_{\pm} = \pm q |X| \qquad (21)$$

$$|\pm\rangle = \frac{1}{\sqrt{2}} \left[\pm \frac{X}{|X|} |3\rangle + |4\rangle \right]. \qquad (22)$$

The matrix elements of spin are also all real by time reversal and non-vanishing only for $\langle \sigma_x \rangle_{33} = -\langle \sigma_x \rangle_{44} \equiv S$ and $\langle \sigma_y \rangle_{34} = \langle \sigma_y \rangle_{43} \equiv T$ and the spin expectation values are zero for σ_x and non-zero for σ_y as

$$\langle \pm | \sigma_y | \pm \rangle = \pm \frac{XT}{|X|} \qquad (23)$$

showing that the spin directions are along y perpendicular to $\boldsymbol{q}$. For $q_x = 0$, $q_y \neq 0$,

$$\varepsilon_{\pm} = \pm q |Y| \qquad (24)$$

$$|+\rangle = |3\rangle, \qquad |-\rangle = |4\rangle, \qquad \text{for } Y > 0 \qquad (25)$$

$$|+\rangle = |4\rangle, \qquad |-\rangle = |3\rangle, \qquad \text{for } Y < 0 \qquad (26)$$

and the spin expectation value of σ_x is S $(-S)$ when the solution is $|3\rangle$ ($|4\rangle$) and the y component becomes zero.

Therefore, the Rashba spin splitting around $\bar{\mathrm{M}}$ may be anisotropic in accordance with the difference between $|X|$ and $|Y|$ and the resulting spin structure may be vortical or non-vortical, governed by the signs in X, Y, S and T. In the Si(111)-($\sqrt{3} \times \sqrt{3}$)–Bi surface, a hyperbolic spin structure is predicted around $\bar{\mathrm{M}}$ [22].

4.5. Other time-reversal degenerate cases

Besides C_{1h}, there exist some other groups where 1D representation states are degenerate by time reversal. The most typical case is a time-reversal pair of Γ_4 and Γ_5 in C_{3v} [24]. By checking the matrix elements with the master equation in equation (7), it is shown that the diagonal and off-diagonal elements of the velocity operator are all zero and that no band splitting linear in q is expected. Nevertheless, the second-order or higher perturbation may remove the degeneracy. The same situation may happen for a time-reversal pair of Γ_6 in C_3. It is shown that a time-reversal pair of Γ_4 and Γ_5 in C_3 can reveal the ideal Rashba effect just like 2D Γ_6 in C_{3v}, however.

5. Summary

By using the $k \cdot p$ perturbation method, it is shown that the velocity-operator term in the perturbation results in the generalized Rashba Hamiltonian. The master equation that the matrix elements of the velocity operator as well as the spin-angular-momentum operator must obey is derived. On the basis of group-theoretical consideration, 2D representation states at $\boldsymbol{k}$ points with the group of k, C_{3v} or C_{4v}, always show the ideal Rashba effect regardless of time reversal. On the other hand, the Rashba effect expected for 2D states belonging to C_{2v} may not be isotropic or vortical, depending on the anisotropic character of the relevant surface states. A time-reversal pair at $\bar{\mathrm{M}}$ with the group of k C_{1h} in the triangular BZ also may reveal possibly anisotropic spin splitting and non-vortical spin structure.

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