

Erratum: Generic model with unconventional Rashba bands and giant spin galvanic effect [Phys. Rev. B **109**, 195419 (2024)]

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Regarding Sec. II A (Hexagonal lattice) of the original paper, we inaccurately described the basis functions of the model. For Sec. II B (Square lattice), the basis functions of the model and its corresponding point group were not clearly introduced and remained ambiguous. Therefore, in this Erratum, we provide a detailed discussion of the basis functions and their symmetry analysis for the respective models. Before proceeding, we clarify two points: First, the unit of the parameter λ_R in the tight-binding model should be eV. Second, the term “hexagonal lattice” is sometimes also referred to as a “trigonal lattice.” This is because, for the C_{3v} point group, it belongs to the trigonal crystal system. Within this system, depending on the lattice choice, some crystals fall under the rhombohedral lattice in the lattice system, while others belong to the hexagonal lattice. In some literature, the term “trigonal lattice” may refer to crystals of the trigonal crystal system.

The tight-binding (TB) models for the hexagonal lattice and the square lattice in the original paper are different; however, their corresponding $\mathbf{k} \cdot \mathbf{p}$ models are identical, as detailed in Sec. II C ($\mathbf{k} \cdot \mathbf{p}$ model) of the original paper. Therefore, we may adopt the $\mathbf{k} \cdot \mathbf{p}$ model for our study. More generally, the intraorbital and interorbital Rashba spin-orbit couplings (SOCs) are not necessarily equal. Thus, the Hamiltonian is written as

$$H = tk^2\tau_0\sigma_0 + \lambda\tau_2\sigma_z + (\lambda_{R1}\tau_0 + \lambda_{R2}\tau_1)(k_x\sigma_y - k_y\sigma_x), \quad (1)$$

where t represents the isotropic kinetic energy term, λ denotes the on-site SOC (intrinsic SOC) strength, and λ_{R1} and λ_{R2} represent the intraorbital and interorbital Rashba SOC strengths, respectively. The orbital and spin degrees of freedom are represented by the Pauli matrices $\boldsymbol{\tau} = (\tau_1, \tau_2, \tau_3)$ and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, respectively, with τ_0 and σ_0 denoting the corresponding 2×2 identity matrices.

For the hexagonal lattice, we consider the constraint of the C_{3v} point group. The C_{3v} point group corresponds to two symmorphic space groups: $P3m1$ (No. 156) and $P31m$ (No. 157). They share the same rotation operations, denoted as C_3^1 and C_3^2 , but differ in their three mirror planes (denoted as σ_v^1 , σ_v^2 , and σ_v^3). As shown in Figs. 1(a) and 1(b), the crystallographic planes of the hexagonal lattice are labeled using Miller-Bravais indices. In the $P3m1$ space group, these three mirror planes are σ_v^1 parallel to the $(11\bar{2}0)$ plane, σ_v^2 parallel to the $(\bar{1}2\bar{1}0)$ plane, and σ_v^3 parallel to the $(2\bar{1}\bar{1}0)$ plane [see Fig. 1(b)]. In the $P31m$ space group, the three mirror planes are σ_v^1 parallel to the $(01\bar{1}0)$ plane, σ_v^2 parallel to the $(\bar{1}100)$ plane, and σ_v^3 parallel to the $(10\bar{1}0)$ plane [see Fig. 1(a)]. We choose the $P31m$ space group to further discuss the basis functions and symmetry of the Hamiltonian [i.e., Eq. (1)].

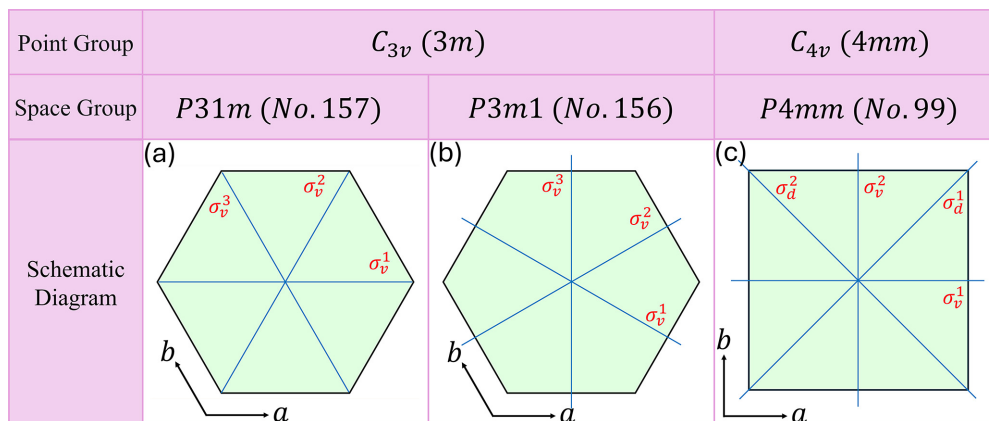


FIG. 1. Schematic diagrams of the symmetry for the two symmorphic space groups under the C_{3v} point group: (a) space group $P31m$ and (b) space group $P3m1$. The difference between them lies in the 30° angular offset in the orientation of the three vertical mirror planes. (c) Schematic diagram of the symmetry for the C_{4v} point group.

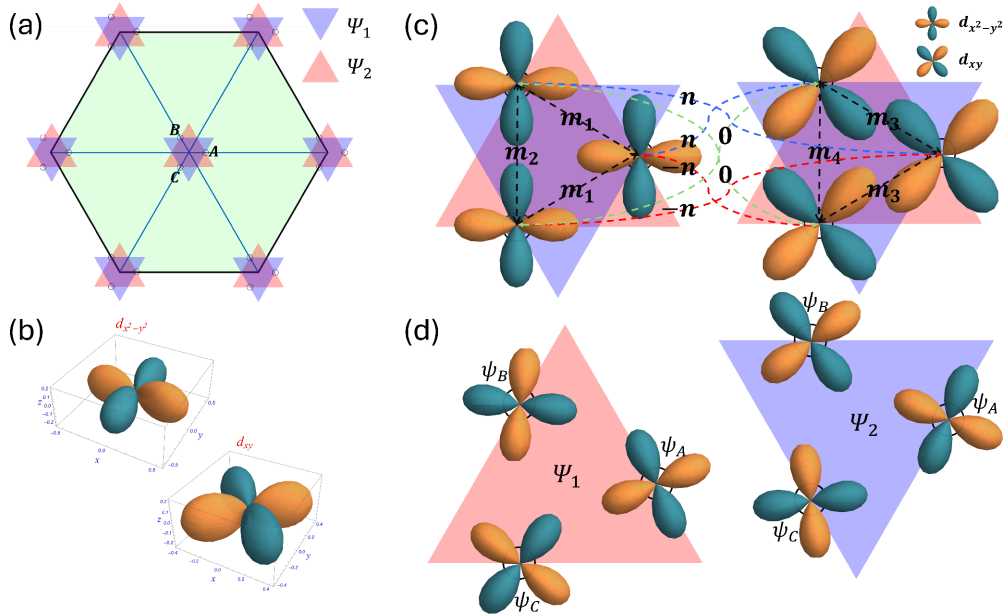


FIG. 2. (a) Schematic of a lattice satisfying the $P31m$ space group. Atoms A, B, and C are identical atoms. Considering the $d_{x^2-y^2}$ and d_{xy} orbitals of each atom, we assume they hybridize to form two orbitals Ψ_1 and Ψ_2 with specific symmetries. (b) Spatial configuration diagrams of the $d_{x^2-y^2}$ and d_{xy} orbitals. (c) Orbital overlap integrals between the $d_{x^2-y^2}$ and d_{xy} orbitals on the three atoms A, B, and C. (d) Orbital configurations ψ_A , ψ_B , and ψ_C at atoms A, B, and C within the Ψ_1 and Ψ_2 orbitals.

For the square lattice, as shown in Fig. 1(c), we consider the constraint of the C_{4v} point group. The four mirror planes are denoted as σ_v^1 , σ_v^2 , σ_d^1 , and σ_d^2 , which are parallel to the planes labeled by Miller indices (010), (100), ($\bar{1}10$), and (110), respectively. In addition to the mirror operations, the rotational operations about the principal axis in the point group are denoted as C_4^1 , C_2 , and C_4^3 .

A. Hexagonal lattice

The C_{3v} point group corresponds to two symmorphic space groups: $P31m$ and $P3m1$. We consider the hexagonal lattice shown in Fig. 2(a), where each lattice site contains three atoms labeled A, B, and C. The positions of these atoms constrain the crystal to belong to the $P31m$ space group. We focus on the $d_{x^2-y^2}$ and d_{xy} orbitals on each atom [Fig. 2(b)], denoted as $d_{x^2-y^2}^A$, d_{xy}^A , $d_{x^2-y^2}^B$, d_{xy}^B , $d_{x^2-y^2}^C$, and d_{xy}^C . These orbitals hybridize to form two new orbitals, labeled Ψ_1 and Ψ_2 . These two orbitals remain invariant under the rotational operations of the C_{3v} point group, but are interchanged under mirror reflections. Therefore, the representation matrices for the orbital part under the symmetry operations of the C_{3v} point group are

$$\begin{aligned} D_{\text{orb}}(E) &= D_{\text{orb}}(C_3^1) = D_{\text{orb}}(C_3^2) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\ D_{\text{orb}}(\sigma_v^1) &= D_{\text{orb}}(\sigma_v^2) = D_{\text{orb}}(\sigma_v^3) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \end{aligned} \quad (2)$$

The representation matrices for the spin degree of freedom under the C_{3v} operations are

$$\begin{aligned} D_{\text{spin}}(E) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad D_{\text{spin}}(C_3^1) = \begin{pmatrix} \omega^* & 0 \\ 0 & \omega \end{pmatrix}, \quad D_{\text{spin}}(C_3^2) = \begin{pmatrix} \omega^{2*} & 0 \\ 0 & \omega^2 \end{pmatrix}, \\ D_{\text{spin}}(\sigma_v^1) &= \begin{pmatrix} 1 & -1 \\ 0 & 0 \end{pmatrix}, \quad D_{\text{spin}}(\sigma_v^2) = \begin{pmatrix} 0 & \omega^2 \\ \omega^{2*} & 0 \end{pmatrix}, \quad D_{\text{spin}}(\sigma_v^3) = \begin{pmatrix} 0 & \omega^{4*} \\ \omega^4 & 0 \end{pmatrix}, \end{aligned} \quad (3)$$

where $\omega = e^{i\pi/3}$. Using the basis $\Phi^\dagger = (c_{\Psi_1, \uparrow}^\dagger, c_{\Psi_1, \downarrow}^\dagger, c_{\Psi_2, \uparrow}^\dagger, c_{\Psi_2, \downarrow}^\dagger)$, the representation matrix for a symmetry operation g in the C_{3v} point group is given by the Kronecker product,

$$D(g) = D_{\text{orb}}(g) \otimes D_{\text{spin}}(g), \quad (4)$$

where $g = E, C_3^1, C_3^2, \sigma_v^1, \sigma_v^2, \sigma_v^3$. We now verify that the Hamiltonian $H(\mathbf{k})$ in Eq. (1) satisfies the symmetry constraint:

$$D^\dagger(g)H(g\mathbf{k})D(g) = H(\mathbf{k}). \quad (5)$$

It is confirmed that this condition holds. Therefore, the new orbitals Ψ_1 and Ψ_2 can serve as the basis functions for the Hamiltonian H in Eq. (1).

Now, we have demonstrated that selecting the new orbitals Ψ_1 and Ψ_2 ensures that the original $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian satisfies the symmetry constraints. For the TB model presented in the original paper, namely the Hamiltonian given by Eq. (13), we can prove that the orbitals Ψ_1 and Ψ_2 remain applicable. Determining the explicit forms of Ψ_1 and Ψ_2 and whether the on-site SOC term can be derived from them are the next steps in our work. We require that Ψ_1 and Ψ_2 satisfy orthogonality and normalization conditions, and that $\Psi_2 = \sigma_v^1 \Psi_1$, where σ_v^1 denotes the mirror operation with respect to the xz plane. Furthermore, we assume that the $d_{x^2-y^2}$ and d_{xy} orbitals on the three atoms A, B, and C satisfy the following relations, as illustrated in Fig. 2(c):

$$\begin{aligned} \text{(i) Normalization:} \quad & \langle d_\mu^i | d_\mu^i \rangle = 1, \quad (\mu \in \{x^2 - y^2, xy\} \text{ and } i \in \{A, B, C\}), \\ \text{(ii) On-site orthogonality:} \quad & \langle d_\mu^i | d_\nu^i \rangle = 0, \quad (\mu \neq \nu \in \{x^2 - y^2, xy\} \text{ and } i \in \{A, B, C\}), \\ \text{(iii) Intersite coupling:} \quad & \langle d_\mu^i | d_\nu^j \rangle = \begin{cases} m_1, & \text{if } \mu = \nu = x^2 - y^2 \text{ and } i \neq j \in \{A, B\}, \\ m_1, & \text{if } \mu = \nu = x^2 - y^2 \text{ and } i \neq j \in \{A, C\}, \\ m_2, & \text{if } \mu = \nu = x^2 - y^2 \text{ and } i \neq j \in \{B, C\}, \\ m_3, & \text{if } \mu = \nu = xy \text{ and } i \neq j \in \{A, B\}, \\ m_3, & \text{if } \mu = \nu = xy \text{ and } i \neq j \in \{A, C\}, \\ m_4, & \text{if } \mu = \nu = xy \text{ and } i \neq j \in \{B, C\}, \\ n, & \text{if } \mu \neq \nu \in \{x^2 - y^2, xy\} \text{ and } i \neq j \in \{A, B\}, \\ -n, & \text{if } \mu \neq \nu \in \{x^2 - y^2, xy\} \text{ and } i \neq j \in \{A, C\}, \\ 0, & \text{if } \mu \neq \nu \in \{x^2 - y^2, xy\} \text{ and } i \neq j \in \{B, C\}, \end{cases} \end{aligned}$$

where m denotes the orbital integral for coupling the same type of orbital at different atomic sites, and n denotes the orbital integral for coupling different types of orbitals at different atomic sites. The different subscripts indicate that the orbital integrals are not necessarily equal.

We assume that the combinations of $d_{x^2-y^2}$ and d_{xy} orbitals on atoms A, B, and C in the Ψ_1 orbital are given by

$$\begin{aligned} \psi_A &= \cos \alpha \cdot d_{x^2-y^2}^A + \sin \alpha \cdot d_{xy}^A, \\ \psi_B &= \cos \left(\alpha + \frac{2\pi}{3} \right) \cdot d_{x^2-y^2}^B + \sin \left(\alpha + \frac{2\pi}{3} \right) \cdot d_{xy}^B, \\ \psi_C &= \cos \left(\alpha + \frac{4\pi}{3} \right) \cdot d_{x^2-y^2}^C + \sin \left(\alpha + \frac{4\pi}{3} \right) \cdot d_{xy}^C, \end{aligned}$$

where the mixing angle α determines the orbital hybridization between the $d_{x^2-y^2}$ and d_{xy} orbitals. The normalization coefficient can be determined from the normalization condition $\langle \Psi_1 | \Psi_1 \rangle = 1$, yielding the expression for the Ψ_1 orbital:

$$\Psi_1 = \frac{1}{\sqrt{\frac{1}{2}(6 - 2m_1 - m_2 - 2m_3 - m_4) + (-m_1 + m_2 + m_3 - m_4 + 2\sqrt{3}n) \cos 2\alpha}} (\psi_A + \psi_B + \psi_C). \quad (6)$$

For the Ψ_2 orbital, under the mirror operation σ_v^1 , the orbital transformation is $d_{x^2-y^2} \mapsto d_{x^2-y^2}$, $d_{xy} \mapsto -d_{xy}$, and the atomic positions transform as $A \mapsto A$, $B \mapsto C$, $C \mapsto B$. Therefore, the combinations of $d_{x^2-y^2}$ and d_{xy} orbitals on atoms A, B, and C in the Ψ_2 orbital are given by

$$\begin{aligned} \psi_A &= \cos \alpha \cdot d_{x^2-y^2}^A - \sin \alpha \cdot d_{xy}^A, \\ \psi_B &= \cos \left(\alpha + \frac{4\pi}{3} \right) \cdot d_{x^2-y^2}^B - \sin \left(\alpha + \frac{4\pi}{3} \right) \cdot d_{xy}^B, \\ \psi_C &= \cos \left(\alpha + \frac{2\pi}{3} \right) \cdot d_{x^2-y^2}^C - \sin \left(\alpha + \frac{2\pi}{3} \right) \cdot d_{xy}^C. \end{aligned}$$

Similar to the derivation for Ψ_1 , we obtain

$$\Psi_2 = \frac{1}{\sqrt{\frac{1}{2}(6 - 2m_1 - m_2 - 2m_3 - m_4) + (-m_1 + m_2 + m_3 - m_4 + 2\sqrt{3}n) \cos 2\alpha}} (\psi_A + \psi_B + \psi_C). \quad (7)$$

After obtaining Ψ_1 and Ψ_2 , through $\langle \Psi_1 | \Psi_2 \rangle$, we find the orthogonality condition to be

$$\langle \Psi_1 | \Psi_2 \rangle = \frac{2(-m_1 + m_2 + m_3 - m_4 + 2\sqrt{3}n) + (6 - 2m_1 - m_2 - 2m_3 - m_4) \cos 2\alpha}{(6 - 2m_1 - m_2 - 2m_3 - m_4) + 2(-m_1 + m_2 + m_3 - m_4 + 2\sqrt{3}n) \cos 2\alpha}, \quad (8)$$

where the two orbitals are orthogonal only when $\alpha = \pm \frac{1}{2} \arccos(-\frac{2(-m_1+m_2+m_3-m_4+2\sqrt{3}n)}{6-2m_1-m_2-2m_3-m_4}) + k\pi$ ($k \in \mathbb{Z}$). Taking $\alpha = \pi/4$, we show the corresponding three orbital components ψ_A , ψ_B , and ψ_C in the Ψ_1 and Ψ_2 orbitals in Fig. 2(d).

Using the new orbitals Ψ_1 and Ψ_2 as the basis, and applying the on-site SOC relations for the atomic $d_{x^2-y^2}$ and d_{xy} orbitals,

$$L_z d_{x^2-y^2} = -2id_{xy}, \quad L_z d_{xy} = 2id_{x^2-y^2}, \quad (9)$$

we obtain

$$\begin{aligned} \langle \Psi_1 | L_z | \Psi_1 \rangle &= 0, \\ \langle \Psi_1 | L_z | \Psi_2 \rangle &= -\frac{6 \sin 2\alpha}{\frac{1}{2}(6-2m_1-m_2-2m_3-m_4) + (-m_1+m_2+m_3-m_4+2\sqrt{3}n) \cos 2\alpha} i, \\ \langle \Psi_2 | L_z | \Psi_1 \rangle &= \frac{6 \sin 2\alpha}{\frac{1}{2}(6-2m_1-m_2-2m_3-m_4) + (-m_1+m_2+m_3-m_4+2\sqrt{3}n) \cos 2\alpha} i, \\ \langle \Psi_2 | L_z | \Psi_2 \rangle &= 0. \end{aligned}$$

We consider the orbital grouping, i.e., the direct product of orbital space and spin space, and write it in matrix form as

$$\begin{aligned} H_{\text{on-site SOC}} &= \lambda \frac{6 \sin 2\alpha}{\frac{1}{2}(6-2m_1-m_2-2m_3-m_4) + (-m_1+m_2+m_3-m_4+2\sqrt{3}n) \cos 2\alpha} \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix} \\ &= \lambda \frac{6 \sin 2\alpha}{\frac{1}{2}(6-2m_1-m_2-2m_3-m_4) + (-m_1+m_2+m_3-m_4+2\sqrt{3}n) \cos 2\alpha} \tau_2 \sigma_z. \end{aligned} \quad (10)$$

If we absorb the factor $\frac{6 \sin 2\alpha}{\frac{1}{2}(6-2m_1-m_2-2m_3-m_4) + (-m_1+m_2+m_3-m_4+2\sqrt{3}n) \cos 2\alpha}$ into λ , we obtain the on-site SOC term in the basis $\Phi^\dagger = (c_{\Psi_1, \uparrow}^\dagger, c_{\Psi_1, \downarrow}^\dagger, c_{\Psi_2, \uparrow}^\dagger, c_{\Psi_2, \downarrow}^\dagger)$ as $\lambda \tau_2 \sigma_z$, which is exactly the on-site SOC term in the Hamiltonian shown in Eq. (1).

Through our calculations and analysis, we demonstrate that the $\mathbf{k} \cdot \mathbf{p}$ model [Eq. (1)] describing the unconventional Rashba bands in the hexagonal lattice satisfies the symmetry constraints of the C_{3v} point group when using the basis $\Phi^\dagger = (c_{\Psi_1, \uparrow}^\dagger, c_{\Psi_1, \downarrow}^\dagger, c_{\Psi_2, \uparrow}^\dagger, c_{\Psi_2, \downarrow}^\dagger)$. It is important to note that our newly derived orbitals Ψ_1 and Ψ_2 are constructed within a three-center system comprising atoms A, B, and C, and this formulation is not applicable to single-atom systems (single-center systems) where the basis consists solely of $d_{x^2-y^2}$ and d_{xy} orbitals.

B. Square lattice

In the case of the hexagonal lattice, the configuration of the three atoms A, B, and C determines its corresponding space group as $P31m$ under the C_{3v} point group. Unlike the hexagonal lattice, describing the square lattice using a three-center system is clearly inappropriate. Therefore, we consider the simplest single-center system, with the corresponding point group being the C_{4v} point group, as shown in Fig. 1(c). Furthermore, we still choose the $d_{x^2-y^2}$ and d_{xy} orbitals of a single atom as the basis for our study.

To verify the symmetry of the Hamiltonian $H(\mathbf{k})$ shown in Eq. (1) under the C_{4v} point group, we consider the transformation matrices for rotational and mirror operations separately and validate the symmetry of $H(\mathbf{k})$ using Eq. (5). Note that it is necessary to consider both the orbital space and the spin space independently, and then take their direct product [as in Eq. (4)], where the basis is now $\Phi^\dagger = (c_{d_{x^2-y^2}, \uparrow}^\dagger, c_{d_{x^2-y^2}, \downarrow}^\dagger, c_{d_{xy}, \uparrow}^\dagger, c_{d_{xy}, \downarrow}^\dagger)$.

For the C_{4v} point group, the group operations g are elements of the set $\{E, C_4^1, C_2, C_4^3, \sigma_v^1, \sigma_v^2, \sigma_d^1, \sigma_d^2\}$. Under rotational operations (which here include the identity operation), i.e., taking $g \in \{E, C_4^1, C_2, C_4^3\}$, we denote the rotation angle about the principal axis (the z axis) as α (taking counterclockwise rotation as positive). The representation matrices for the group operation acting on $\mathbf{k} = (k_x, k_y)$, the orbitals $d_{x^2-y^2}$ and d_{xy} , and the spin are respectively given by

$$D(\alpha, \mathbf{k}) = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} k_x \\ k_y \end{pmatrix} = \begin{pmatrix} k_x \cos \alpha - k_y \sin \alpha \\ k_x \sin \alpha + k_y \cos \alpha \end{pmatrix}, \quad (11)$$

$$D_{\text{orb}}(\alpha) = e^{-2i\tau_2 \alpha} = \begin{pmatrix} \cos 2\alpha & -\sin 2\alpha \\ \sin 2\alpha & \cos 2\alpha \end{pmatrix}, \quad (12)$$

$$D_{\text{spin}}(\alpha) = e^{-i\sigma_z \alpha/2} = e^{-i\sigma_z \alpha/2} = \begin{pmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{pmatrix}. \quad (13)$$

Further, using Eqs. (4) and (5), we obtain the transformed Hamiltonian under the group operation as

$$\begin{aligned} H' &= t k^2 \tau_0 \sigma_0 + \lambda \tau_2 \sigma_z + [\lambda_{R1} \tau_0 + \lambda_{R2} (\tau_1 \cos 4\alpha + \tau_3 \sin 4\alpha)] (k_x \sigma_y - k_y \sigma_x) \\ &= H + \lambda_{R2} [\tau_1 (\cos 4\alpha - 1) + \tau_3 \sin 4\alpha] (k_x \sigma_y - k_y \sigma_x). \end{aligned} \quad (14)$$

We observe that for $H' = H$ to hold, α must satisfy $\alpha = k\frac{\pi}{2}$, where $k \in \mathbb{Z}$. For the rotational operations considered here, namely $g \in E, C_4^1, C_2, C_4^3$, the corresponding rotation angles are $\alpha = 0, \pi/2, \pi$, and $3\pi/2$, respectively. Therefore, the original Hamiltonian $H(\mathbf{k})$ satisfies the rotational symmetry under the C_{4v} point group.

Under mirror operations, where $g \in \{\sigma_v^1, \sigma_v^2, \sigma_d^1, \sigma_d^2\}$, we define the angle between the mirror plane and the x axis as β (taking the counterclockwise rotation from the x axis to the mirror plane as positive). The representation matrices for the group operation acting on $\mathbf{k} = (k_x, k_y)$, the orbitals $d_{x^2-y^2}$ and d_{xy} , and the spin are respectively given by

$$D(\beta, \mathbf{k}) = \begin{pmatrix} \cos 2\beta & \sin 2\beta \\ \sin 2\beta & -\cos 2\beta \end{pmatrix} \begin{pmatrix} k_x \\ k_y \end{pmatrix} = \begin{pmatrix} k_x \cos 2\beta + k_y \sin 2\beta \\ k_x \sin 2\beta - k_y \cos 2\beta \end{pmatrix}, \quad (15)$$

$$D_{\text{orb}}(\beta) = \begin{pmatrix} \cos 4\beta & \sin 4\beta \\ \sin 4\beta & -\cos 4\beta \end{pmatrix}, \quad (16)$$

$$D_{\text{spin}}(\beta) = e^{-i(\mathbf{n} \cdot \boldsymbol{\sigma})\pi/2} = e^{-i(-\sin \beta \sigma_x + \cos \beta \sigma_y)\pi/2} = \begin{pmatrix} 0 & -e^{-i\beta} \\ e^{i\beta} & 0 \end{pmatrix}. \quad (17)$$

Following a similar approach to the rotation operation and using Eqs. (4) and (5), we obtain the transformed Hamiltonian under mirror operation as

$$\begin{aligned} H'' &= tk^2\tau_0\sigma_0 + \lambda\tau_2\sigma_z + [\lambda_{R1}\tau_0 + \lambda_{R2}(-\tau_1 \cos 8\beta + \tau_3 \sin 8\beta)](k_x\sigma_y - k_y\sigma_x) \\ &= H + \lambda_{R2}[-\tau_1(\cos 8\beta + 1) + \tau_3 \sin 8\beta](k_x\sigma_y - k_y\sigma_x). \end{aligned} \quad (18)$$

At this point, if we require the transformed Hamiltonian to be equal to the original Hamiltonian, i.e., $H'' = H$, we obtain $\beta = \frac{\pi}{8} + k\frac{\pi}{4}$, where $k \in \mathbb{Z}$. For $g \in \{\sigma_v^1, \sigma_v^2, \sigma_d^1, \sigma_d^2\}$, the corresponding values of β are $0, \pi/2, \pi/4$, and $3\pi/4$, respectively. We find that these values are not within the solution set for β that we derived. Therefore, the original Hamiltonian $H(\mathbf{k})$ does not possess mirror symmetry in the basis of $d_{x^2-y^2}$ and d_{xy} orbitals. Nevertheless, we observe that if the mirror plane is shifted by $\pi/8$, then $H'' = H$ holds. This indicates that our choice of basis is incompatible with the C_{4v} point group. Since the derived Hamiltonians H' and H'' contain τ_3 -related terms, we can propose a new Hamiltonian:

$$\tilde{H} = tk^2\tau_0\sigma_0 + \lambda\tau_2\sigma_z + (\lambda_{R1}\tau_0 + \lambda_{R2}\tau_3)(k_x\sigma_y - k_y\sigma_x). \quad (19)$$

This Hamiltonian eliminates the interorbital Rashba SOC, but introduces different intraorbital Rashba SOC strengths for the two distinct orbitals.

For the new Hamiltonian $\tilde{H}(\mathbf{k})$, we still choose $\Phi^\dagger = (c_{d_{x^2-y^2}, \uparrow}^\dagger, c_{d_{x^2-y^2}, \downarrow}^\dagger, c_{d_{xy}, \uparrow}^\dagger, c_{d_{xy}, \downarrow}^\dagger)$ as the basis. Applying rotational symmetry using Eqs. (11)–(13), we obtain

$$\begin{aligned} \tilde{H}' &= tk^2\tau_0\sigma_0 + \lambda\tau_2\sigma_z + [\lambda_{R1}\tau_0 + \lambda_{R2}(-\tau_1 \sin 4\alpha + \tau_3 \cos 4\alpha)](k_x\sigma_y - k_y\sigma_x) \\ &= \tilde{H} + \lambda_{R2}[-\tau_1 \sin 4\alpha + \tau_3(\cos 4\alpha - 1)](k_x\sigma_y - k_y\sigma_x). \end{aligned} \quad (20)$$

Applying mirror symmetry using Eqs. (15)–(17), we obtain

$$\begin{aligned} \tilde{H}'' &= tk^2\tau_0\sigma_0 + \lambda\tau_2\sigma_z + [\lambda_{R1}\tau_0 + \lambda_{R2}(\tau_1 \sin 8\beta + \tau_3 \cos 8\beta)](k_x\sigma_y - k_y\sigma_x) \\ &= \tilde{H} + \lambda_{R2}[\tau_1 \sin 8\beta + \tau_3(\cos 8\beta - 1)](k_x\sigma_y - k_y\sigma_x). \end{aligned} \quad (21)$$

The solution to Eq. (20) is $\alpha = k\frac{\pi}{2}$, where $k \in \mathbb{Z}$. It is evident that this solution is identical to that of Eq. (14), indicating that $\tilde{H}$ possesses rotational symmetry. The solution to Eq. (21) is $\beta = k\frac{\pi}{4}$, where $k \in \mathbb{Z}$. It can be observed that this now encompasses the values $0, \pi/2, \pi/4$, and $3\pi/4$. Therefore, $\tilde{H}$ also exhibits mirror symmetry.

The Hamiltonians H and $\tilde{H}$ are unitarily equivalent through the transformation

$$H = U_{\text{total}}^\dagger \tilde{H} U_{\text{total}}, \quad (22)$$

where $U_{\text{total}} = U \otimes \sigma_0$ with $U = e^{i\pi\tau_2/4} = \frac{1}{\sqrt{2}}(\tau_0 + i\tau_2)$ acting solely on the orbital space. Given that $\tilde{H}$ is expressed in the basis $\Phi^\dagger = (c_{d_{x^2-y^2}, \uparrow}^\dagger, c_{d_{x^2-y^2}, \downarrow}^\dagger, c_{d_{xy}, \uparrow}^\dagger, c_{d_{xy}, \downarrow}^\dagger)$, the basis for H is transformed as $\Phi^\dagger U_{\text{total}}$, yielding the explicit new basis $\Phi^\dagger = \frac{1}{\sqrt{2}}(c_{d_{x^2-y^2}, \uparrow}^\dagger - c_{d_{xy}, \uparrow}^\dagger, c_{d_{x^2-y^2}, \downarrow}^\dagger - c_{d_{xy}, \downarrow}^\dagger, c_{d_{x^2-y^2}, \uparrow}^\dagger + c_{d_{xy}, \uparrow}^\dagger, c_{d_{x^2-y^2}, \downarrow}^\dagger + c_{d_{xy}, \downarrow}^\dagger)$. This corresponds to a rotation in orbital pseudospin space, mapping the original τ_3 eigenstates to eigenstates of τ_1 . The transformation preserves all terms except the λ_{R2} Rashba SOC, which transforms as

$$U^\dagger(\lambda_{R2}\tau_3)U = \lambda_{R2}\tau_1, \quad (23)$$

while the kinetic term $tk^2\tau_0\sigma_0$, on-site SOC $\lambda\tau_2\sigma_z$, and λ_{R1} Rashba SOC remain invariant. This establishes the complete physical equivalence between the two representations.

Correction: Typographical errors in Eqs. (22) and (23) as well as in an expression in the text following Eq. (22) have been fixed.