An upper and lower bound to the orientation-dependent linear Rashba spin-orbit coupling of two-dimensional hole gases in semiconductor quantum wells

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Our recent study [Phys. Rev. B 103, 085309 (2021)] verified the existence of $k$-linear Rashba spin-orbit coupling (SOC) of two-dimensional hole gases in quantum wells (QWs) which originates from a combination of heavy-hole-light-hole (HH-LH) mixing and direct dipolar coupling to the external electric field. However, the Rashba SOC dependence on QW orientations remains unclear. Here, we explore this dependence on QW orientations and uncover an upper and lower bound to the orientation-dependent $k$-linear Rashba SOC along the [110]- and [111]-crystalline directions by performing atomistic pseudopotential calculations associated with theoretical analysis. The intrinsic HH-LH mixing at the Brillouin zone center, maximal in [110]-oriented quantum wells and minimal in [111]- and [001]-oriented QWs, plays an essential role. Remarkably, we find that only $k$-cubic Rashba SOC exists in [111]-oriented QWs. These findings help understand the physical mechanism of the Rashba SOC dependence on QW orientations and provide a strategic prediction for experiments to realize the large Rashba SOC.

I. INTRODUCTION

Spin-orbit coupling (SOC) provides the use of the spin degree of freedom for information creation, manipulation, and detection, wherein the Rashba SOC realizes the electric control of spins due to the breaking of structural inversion symmetry.1–2 Recently, extensive research attention in SOC has been centralized at hole spins, because holes have weaker hyperfine interaction compared to electrons and thus have much longer spin dephasing time.3–6 Since group III-V semiconductors, such as InAs and GaAs, have strong nuclear spins, which interact with hole spins and leads to short spin dephasing time, practical applications are difficult for these materials. Correspondingly, group IV semiconductors, such as Ge and Si, have abundant isotopes with zero nuclear spins and can be further isotopically purified to produce long spin dephasing time.7,8 More importantly, Ge and Si have mature microelectronic technologies and are compatible with Complementary-Metal-Oxide-Semiconductor (CMOS), and Ge has the largest hole mobility among all known semiconductors. Very recently, Hendrickx et al. implemented fast single and two spin-qubit logic with holes in planar Ge8, where the fast spin manipulation gives the credit to the strong SOC9–11. All these factors jointly push Ge and Si into the center stage of semiconductor spintronics and solid quantum devices.

Two-dimensional (2D) semiconductor quantum wells (QWs) with SOC are a promising platform for a vast number of physical effects and device applications, such as spin Hall effect12–14, spin galvanic effect15–17, spin transistors18,19, and spin qubits20. Based on different applications, strong or weak Rashba SOC in QWs is desirable to satisfy corresponding requirements. On the one hand, for example, strong Rashba SOC is highly demanded for one-qubit operations, because it can manipulate the qubit very fast by the electric dipole spin resonance (EDSR), which is an all-electrical method.20–24 On the other hand, weak Rashba SOC is required for some cases. For example, strong Rashba SOC may involve the electrical noises via entangling the spins and orbitals, leading to spin decoherence.25 For two-qubit quantum dot systems, strong SOC is the dominant spin-mixing mechanism giving rise to the unwanted leakage current.26 Therefore, for these cases, weak Rashba SOC is preferred. Our recent study found a first-order $k$-linear Rashba SOC in two-dimensional hole gases (2DHGs) in Ge/Si QWs, which originates from a combination of heavy-hole-light-hole (HH-LH) mixing and direct dipolar coupling to the external electric field27. We found that the Rashba SOC in [110]-oriented QWs is much stronger than [001]-oriented QWs, where the largest Rashba SOC can reach 120 meV/Å27. The tunable range of Rashba SOC in these two QW orientations differs to reach two orders of magnitudes, inspiring us that the QW orientation plays a significant role in strong or weak Rashba SOC. In the one-dimensional (1D) case, Kloeffel et al. systematically studied the low-energy states and the direct Rashba SOC in Si and Ge nanowires with different growth directions23, but the study of the Rashba SOC in 2D QWs grown in different directions remains void. Most experimental and theoretical researches in spin physics spotlight on [001]-oriented QWs28–32, though researchers studied the intersubband infrared absorption in the [110]-oriented Si/Si$_x$Ge$_{1-x}$ QWs33,34 and quantum cascade lasers in [111]-oriented Si/SiGe QWs35. No systematic researches focus on the Rashba SOC in QWs with different orientations. One would naturally raise the question of how the QW orientation determines the Rashba SOC, whether we could find a strong or weak Rashba SOC in QWs grown in other directions except for [110] and [001].
crystalline directions, and which direction could produce the strongest or the weakest Rashba SOC.

In this paper, we study the Rashba SOC of 2DHGs in Ge/Si QWs grown in different directions by using the atomistic semiempirical pseudopotential method (SEPM)\textsuperscript{36–38}, and confirm the upper and lower bound to the orientation-dependent k-linear Rashba SOC with [110] and [111] crystalline directions, respectively. By doing the transformation of the Luttinger-Kohn (LK) Hamiltonian, we illustrate that the intrinsic HH-LH mixing, as the dominant factor, has the maximum and minimum in [110] and [111] crystalline directions. We reveal that only k-cubic Rashba SOC exists in [111]-oriented QWs because the HH-LH mixing is forbidden by symmetry, and further examine the field- and size-dependencies of k-cubic Rashba parameters $\gamma_R$. One can choose QWs grown in [111] direction or other directions to obtain the k-cubic or k-linear Rashba SOC.

This paper is organized as follows. In Sec. II, we introduce the computational method SEPM for obtaining the spin splitting and Rashba parameters. In the results shown in Sec. III, we first show the k-linear Rashba SOC of 2DHGs for QWs grown in different directions, illustrating the importance of HH-LH mixing. We next do the transformation of LK Hamiltonian and show the HH-LH mixing dependence on QW orientations, which determines the strength of the k-linear Rashba SOC. We then show the k-cubic Rashba SOC in [111]-oriented QWs, and explain this interesting phenomenon from the perspective of symmetry. We also explore the electric-field- and size-dependencies of this k-cubic Rashba SOC. In Sec. IV, we give a discussion and summarize our conclusion.

II. COMPUTATIONAL METHODS

The SEPM calculation uses a supercell approach with a periodic boundary condition, where the supercell of one Ge/Si QW consists of $1 \times 1 \times (m+n)$ atomic layers ($m$ and $n$ are Ge and Si thickness in atomic layers). We adopt the valence force field (VFF) approach, which has been widely applied to semiconductor nanostructures\textsuperscript{39–46}, to minimize the strain energy in Ge/Si QWs produced by the 4.2 \% lattice mismatch. All the Ge/Si QWs show a 1 \% compressive strain occurred in the Ge well and a 3 \% tensile strain in the Si barrier. After the VFF relaxation, we use the atomistic SEPM accompanied with a plane-wave basis set and folded-spectrum diagonalization\textsuperscript{47}, which has been successfully used to study semiconductor superstructure\textsuperscript{43–45,48–53}, to calculate the electronic structure of QWs. The crystal potential of QWs superposes the screened atomic potentials, which include a local part and a non-local spin-orbit interaction part. The atomic potentials were obtained by fitting to reproduce experimental transition energies, effective masses, spin-orbit splittings, and deformation potentials of the bulk semiconductors to remove the “LDA” error\textsuperscript{37,38}. We use an energy cutoff of 8.2 Ry to select the plane-wave basis and use the fast Fourier transformation to transform the wave function between a reciprocal space grid and a real-space grid. We use a $16 \times 16 \times 16$ grid in real space for each eight-atom cubic cell\textsuperscript{37,38}. Our SEPM results of the Rashba parameters, including the k-linear and k-cubic ones ($\alpha_R$ and $\gamma_R$), are obtained by fitting the spin splitting near the $\bar{\Gamma}$ point: $\Delta E_{\text{ss}} = 2\alpha_R k + \gamma_R k^3$, where we directly solve the Shrödinger equation with an applied perpendicular electric field to obtain the band structure and spin splitting.

III. RESULTS

A. Linear Rashba effect in 2DHGs of QWs with different orientations

Fig. 1(a) shows the spin splitting obtained from the SEPM calculated valence band structure of [110]-, [111]-, [112]-, [113]-, [114]- and [001]-oriented Ge/Si QWs under a perpendicular electric field of 100 kV/cm. The subbands are spin-degenerated at the $\bar{\Gamma}$ point due to the time-reversal symmetry (Kramer’s degeneracy), and split away from the $\bar{\Gamma}$ point, giving rise to the spin splitting. The Ge/Si QWs are type-II QWs, where the electrons are confined in Si layers and the holes are confined in Ge layers because the bulk Ge has a 500 meV higher valence band maximum (VBM) than the bulk Si\textsuperscript{54}. The spin splitting near the $\bar{\Gamma}$ point is entirely induced by the external electric field and interfaces (Rashba ef-
fect\textsuperscript{55}, because the inversion symmetry (Dresselhaus effect\textsuperscript{56}) is absent in Ge and Si bulk crystals. We find that the spin splittings of \([110]\)-, \([112]\)-, \([113]\)-, \([114]\)-, \([001]\)-oriented QWs exhibit a nice \(k\)-linear relationship near the \(\bar{\Gamma}\) point. This \(k\)-linear spin splitting, as illustrated in our recent study\textsuperscript{27}, originates from the HH-LH mixing at the \(\bar{\Gamma}\) point and direct dipolar coupling to the external electric field. However, the spin splitting of the \([111]\)-oriented QW possesses a \(k\)-cubic relationship with the value comparable to the \([001]\)-oriented QW [Fig. 1(b)], which we will explain in the following part. By fitting the spin splitting \(\Delta E_{\alpha\beta} = 2\alpha_R k + \gamma_R k^3\), we obtain the \(k\)-linear and \(k\)-cubic Rashba parameters (\(\alpha_R\) and \(\gamma_R\)): \(\alpha_R = 82, 49, 33, 15, 3\) meV for \([110]\)-, \([112]\)-, \([113]\)-, \([114]\)-, and \([001]\)-oriented QWs, and \(\gamma_R = 23732\) meV Å\(^3\) for \([111]\)-oriented QWs. The \(k\)-linear Rashba parameter \(\alpha_R\) has the maximum (minimum) for the \([110]\)-oriented (\([111]\)-oriented) QW.

We compare the \(k\)-linear Rashba parameter \(\alpha_R\) of QWs grown in different directions in Fig. 2 by including the influence of electric field and size. The upper and lower bound to the \(k\)-linear Rashba parameters \(\alpha_R\) appear in \([110]\) and \([111]\) crystalline orientations, respectively. For \([mnm]\) crystalline orientations (\(n > m\)), the \(k\)-linear Rashba parameter \(\alpha_R\) decreases with the increasing Miller index \(n\). This relationship keeps basically unchanged when one changes the electric field and well thickness. As shown in Fig. 2(b), the electric field has the same strength 100 kV/cm, thus the direct dipolar coupling contributes similarly to different oriented QWs. Consequently, the HH-LH mixing at the \(\bar{\Gamma}\) point is the critical factor to determine the Rashba parameters in QWs with different orientations.

The zone-center HH-LH mixing in QWs includes two parts. The first part arises from the breaking of the axial symmetry\textsuperscript{54}. This HH-LH mixing is irrelevant to both the heterostructure interface and external electric field, and only relies on the QW orientation. Winkler pointed out that the HH-LH mixing usually exists in QWs grown in low-symmetry directions\textsuperscript{54}. Here we call this mixing the intrinsic HH-LH mixing. The second part is the HH-LH mixing induced by the heterostructure interface and the external electric field. To distinguish this HH-LH mixing from the intrinsic HH-LH mixing, we call this mixing the extrinsic HH-LH mixing. We have discussed these two mixings in \([001]\)- and \([110]\)-oriented Ge/Si QWs in our previous work\textsuperscript{27}. The intrinsic HH-LH mixing remains zero in \([001]\)-oriented QWs, but exists in \([110]\)-oriented QWs with the value of

\[ C_{in}^{[110]} = \frac{\sqrt{3}}{2} \left| \gamma_2 - \gamma_3 \right|, \]  

where \(\gamma_1, \gamma_2\) and \(\gamma_3\) are the Luttinger parameters (we give the derivation in the following part). Thus, the \(k\)-linear Rashba SOC in the \([001]\)-oriented QW is completely produced by the extrinsic HH-LH mixing, whereas the Rashba SOC in the \([110]\)-oriented QW is produced by both the intrinsic and extrinsic HH-LH mixing. However, the Rashba parameter in the \([001]\)-oriented QW, compared to that in the \([110]\)-oriented QW, is quite small (Fig. 2). In other words, the extrinsic HH-LH mixing, compared to the intrinsic HH-LH mixing, is negligible\textsuperscript{54}, and the intrinsic HH-LH mixing is dominant. This is consistent with the physical image that the hole wave-function, whose integration gives rise to the Rashba parameter, distributes dominantly in the well but little at the interface.

B. Hamiltonian transformation and intrinsic HH-LH mixing in QWs

We then unravel the intrinsic HH-LH mixing in QWs with different orientations. We do this by transforming the bulk LK Hamiltonian, which describes valence bands well, into different \(z\) directions. The LK Hamiltonian\textsuperscript{97} is written as

\[ H_{LK} = \frac{\hbar^2}{2m}[(\gamma_1 + \frac{5}{2} \gamma_2)(k_x^2 + k_y^2 + k_z^2) - 2\gamma_2(k_x^2 J_{x'} + k_y^2 J_{y'} + k_z^2 J_{z'}) - 4\gamma_3\{k_x' k_y' J_{x'}, J_{y'}\} + \{k_y', k_z'\} \{J_{y'}, J_{z'}\} + \{k_z', k_x'\} \{J_{z'}, J_{x'}\})], \]
where $\hbar$ is the reduced Plank constant, $m^*$ is the effective mass of holes, $k_i$ ($i = x', y', z'$) are the wave vectors, $J_i$ ($i = x', y', z'$) are the hole effective spin operators, $x' || [100]$, $y' || [010]$, $z' || [001]$, and $\{ \mathbf{A}, \mathbf{B} \} = \frac{\mathbf{A} \mathbf{B} + \mathbf{B} \mathbf{A}}{2}$.

To transform the coordinate system, we use the SO(3) rotation groups

$$
\hat{R}(\alpha, \beta, \gamma) = 
\begin{pmatrix}
\cos \alpha \cos \beta \cos \gamma - \sin \alpha \sin \gamma & -\cos \alpha \cos \beta \sin \gamma - \sin \alpha \cos \gamma & \cos \alpha \sin \beta \\
\sin \alpha \cos \beta \cos \gamma + \cos \alpha \sin \gamma & -\sin \alpha \cos \beta \sin \gamma + \cos \alpha \cos \gamma & \sin \alpha \sin \beta \\
-\sin \beta \cos \gamma & -\sin \beta \sin \gamma & \cos \beta 
\end{pmatrix},
$$

where $\alpha$ ($0 \leq \alpha \leq 2\pi$), $\beta$ ($0 \leq \beta \leq \pi$) and $\gamma$ ($0 \leq \gamma \leq 2\pi$) are the Euler angles denoting the rotation angles in order of the $z'$, $y'$ and $z'$ axes. We then obtain the transformed $k_i$ ($i = x, y, z$)

$$
k_{x'} = [(\mathbf{R}^{-1})^T]_{11}k_x + [(\mathbf{R}^{-1})^T]_{12}k_y + [(\mathbf{R}^{-1})^T]_{13}k_z \\
k_{y'} = [(\mathbf{R}^{-1})^T]_{21}k_x + [(\mathbf{R}^{-1})^T]_{22}k_y + [(\mathbf{R}^{-1})^T]_{23}k_z \\
k_{z'} = [(\mathbf{R}^{-1})^T]_{31}k_x + [(\mathbf{R}^{-1})^T]_{32}k_y + [(\mathbf{R}^{-1})^T]_{33}k_z,
$$

and the transformed $J_i$ ($i = x, y, z$)

$$
J_{x'} = [(\mathbf{R}^{-1})^T]_{11}J_x + [(\mathbf{R}^{-1})^T]_{12}J_y + [(\mathbf{R}^{-1})^T]_{13}J_z \\
J_{y'} = [(\mathbf{R}^{-1})^T]_{21}J_x + [(\mathbf{R}^{-1})^T]_{22}J_y + [(\mathbf{R}^{-1})^T]_{23}J_z \\
J_{z'} = [(\mathbf{R}^{-1})^T]_{31}J_x + [(\mathbf{R}^{-1})^T]_{32}J_y + [(\mathbf{R}^{-1})^T]_{33}J_z.
$$

We insert Eq. (4, 5) into Eq. (2) and then obtain the transformed LK Hamiltonian in the form of the Euler angles $\alpha$, $\beta$ and $\gamma$. Because we care the intrinsic HH-LH mixing at $\Gamma$ point and the quantum well (QW) is confined along with the $z$ direction, we set $k_z = k_y = 0$ and $k_z = \frac{\pi}{L}$ ($L$ denotes the well thickness) in this Hamiltonian. In the basis of $|J^2, J_z\rangle = \{|\frac{3}{2}, \frac{3}{2}\rangle, |\frac{3}{2}, -\frac{3}{2}\rangle, |\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle\}$, the Hamiltonian matrices are...
\[
\begin{align*}
\langle H_{LK} \rangle_{11} &= \frac{\pi^2\hbar^2 [32\gamma_1 - 31\gamma_2 - 33\gamma_3 - 3(\gamma_2 - \gamma_3)(4\cos 2\beta + 7\cos 4\beta + 8\cos 4\alpha \sin^4 \beta)]}{64m^*L^2}, \\
\langle H_{LK} \rangle_{12} &= 0, \\
\langle H_{LK} \rangle_{13} &= \frac{\sqrt{3}\pi^2\hbar^2(\gamma_2 - \gamma_3)e^{i\gamma} \sin \beta[(9 - \cos 4\alpha) \cos \beta + (7 + \cos 4\alpha) \cos 3\beta - 4i \sin 4\alpha \sin^2 \beta]}{16m^*L^2}, \\
\langle H_{LK} \rangle_{14} &= -\frac{\sqrt{3}\pi^2\hbar^2(\gamma_2 - \gamma_3)e^{2i\gamma} \sin^2 \beta[5 + 7 \cos 2\beta + \cos 4\alpha(3 + \cos 2\beta) + 4i \cos \beta \sin 4\alpha]}{16m^*L^2},
\end{align*}
\]

where \(\gamma_1, \gamma_2\) and \(\gamma_3\) are the Luttinger parameters.

We then obtain the intrinsic HH-LH mixing independent of the well thickness

\[
C_{in} = \frac{|\langle H_{LK} \rangle_{14}|}{\sqrt{\langle H_{LK} \rangle_{11}^2 + \langle H_{LK} \rangle_{12}^2 + \langle H_{LK} \rangle_{13}^2 + \langle H_{LK} \rangle_{14}^2}}
\]

We note that the coordinate transformation [Eq. (2-7)] brings in the Euler angles \(\alpha, \beta, \gamma\) for process description. As illustrated in Fig. 3(a), we need three steps to transform the initial coordinate system into the final coordinate system: (i). rotation around the z-axis with \(\alpha\) angle \((0 \leq \alpha \leq 2\pi)\); (ii). rotation around the y-axis with \(\beta\) angle \((0 \leq \beta \leq \pi)\); (iii). rotation around the z-axis with \(\gamma\) angle \((0 \leq \gamma \leq 2\pi)\). We note that the first two steps with \(\alpha\) and \(\beta\) angle involved already determine the finally-transformed z-axis, and the last step related to \(\gamma\) angle only determines the x- and y-axis in the x-y plane. Hence we study the intrinsic HH-LH mixing as a function of \(\alpha\) and \(\beta\) angles [the correspondence between the Euler angles and QW orientations are listed in the inset table of Fig. 3(d)] and show the results in Fig. 3(b).

For \([001]\) (\(\beta = 0\)) and \([111]\)-oriented QWs \((\alpha = \pi/4, \beta = \arccos \sqrt{3}/3)\), the intrinsic HH-LH mixing remains zero. For \([110]\)-oriented QWs \((\alpha = \pi/4, \beta = \pi/2)\) the intrinsic HH-LH mixing reduces to Eq. (1).

Fig. 3(b) depicts that: (i). The largest intrinsic HH-LH mixing appears in the \([110]\) crystalline orientation (denoted in dark blue); (ii). The smallest intrinsic HH-LH mixing appears in the \([111]\) and \([001]\) crystalline orientations (denoted in shallow yellow); (iii). Along with the \([mnm]\) crystalline orientation (denoted as the dashed line), as also shown in Fig. 3(c), the intrinsic HH-LH mixing decreases from \([110]\) (maximum) to \([111]\) crystalline orientation (minimum, no mixing), increases from \([111]\) to \([112]\) crystalline orientation approximately, and decreases from \([112]\) to \([001]\) crystalline orientation (minimum, no mixing). Fig. 3(d) presents the intrinsic HH-LH mixing with different QW orientations corresponding to the \(k\)-linear Rashba parameters in Fig. 2, showing a perfect consistency of the orientation-dependence, including the upper and lower bound in \([110]\) and \([111]\) crystalline orientations, respectively. This consistency further confirms the intrinsic HH-LH mixing as the dominant factor of \(k\)-linear Rashba parameters.

However, by comparing the \(k\)-linear Rashba parameters (Fig. 2) and the intrinsic HH-LH mixing (Fig. 3(d)), we note that the Rashba parameter exists in \([001]\)-oriented QWs but vanishes in \([111]\)-oriented QWs, though no intrinsic HH-LH mixing exists in both of these two crystalline orientations. Since the heterostructure interface and the external electric field, as we mentioned above, induce the extrinsic HH-LH mixing and thus lead to the emergence of \(k\)-linear Rashba parameters in \([001]\)-oriented QWs, one may naturally raise the question that why the interface and the external electric field fail to induce the intrinsic HH-LH mixing in \([111]\)-oriented QWs. To answer this question, we have to understand the symmetry requirement from the perspective of group theory, which we will discuss in the following part.

C. Cubic Rashba effect of 2DHGs in \([111]\)-oriented QWs

To confirm the relationship between the spin splitting and the wave vector near the \(\bar{\Gamma}\) point, we extract the

![FIG. 4: Calculated k-cubic hole Rashba parameters \(\gamma_R\) in \([111]\)-oriented QWs as a function of (a) electric field strength with 48 ML well thickness, and (b) well thickness (the red line) and band gap (the blue line) under an electric field of 100 kV/cm, respectively. The Si thickness is 24 ML.](https://example.com/figure4.png)
spin splitting from our SEPM calculated band structure in the [111]-oriented Ge$_{48}$/Si$_{24}$ QW, and find a k-cubic Rashba spin splitting [the red line in Fig. 1(b)], with the k-cubic Rashba parameter $\gamma_R$ of 23732 meVÅ$^3$. This k-cubic spin splitting in the [111]-oriented Ge$_{48}$/Si$_{24}$ QW is comparable to the k-linear spin splitting in the [001]-oriented Ge$_{48}$/Si$_{24}$ QW [the blue line in Fig. 1(b)], where the k-linear Rashba parameter $\alpha_R$ is 2 meVÅ. We also note that the k-cubic Rashba parameter $\gamma_R$ is comparable to the experimentally measured results, including 226000 meVÅ$^3$ for strained Ge/SiGe QWs$^{32}$ and 2000 meVÅ$^3$ for SrTiO$_3$ interfaces$^{56}$.

We further examine the field- and size-dependencies of k-cubic Rashba parameters $\gamma_R$ in [111]-oriented QWs. Fig. 4(a) shows that $\gamma_R$ has a linear scale as $E_z$, satisfying the theoretical prediction of linear-in-field in k-cubic Rashba parameters$^{54}$. Under a fixed electric field $E_z=100$ kV/cm with varying well thickness, as shown in Fig. 4(b), $\gamma_R$ increases linearly against the well thickness when $L < 48$ ML, and increases at a much slower rate till almost saturation when $L > 48$ ML (the red line). This is because the band gap decreases with increasing well thickness and gradually saturates [the blue line shown in Fig. 4(b)] due to the reduced quantum confinement effect, leading to k-cubic Rashba parameters $\gamma_R$, which is inversely proportional to the squared bandgap ($\propto 1/E_g^2$)$^{54}$, to increase till saturation.

This emergence of k-cubic Rashba SOC of 2DHGs in [111]-oriented QWs is rather interesting. The symmetry of interface along [111] crystalline direction forbids the HH-LH mixing, leading to the vanishing of the k-linear Rashba SOC as a result of zero HH-LH mixings. We list the double point groups without interfaces and one of interfaces with corresponding irreducible representations of HH and LH states in QWs grown in different directions in Table I$^{54,59,60}$ to further illustrate this point. For [001]-oriented QWs, the heterostructure interface reduces the symmetry from $D_{2d}$ to $C_{2v}$ due to the lack of microscopic translational symmetry induced by the different atom types at the two sides of the interface$^{54,59}$, resulting in the change of different representations for HH and LH states ($\Gamma_5$ and $\Gamma_7$ as shown in Table I) into the same $\Gamma_3$ representation for both HH and LH states and hence the allowance of HH-LH mixing. For [110]- and [111]-oriented QWs, however, the symmetry keeps invariant no matter we consider the interface or not. The symmetry of [110]-oriented QWs is also $C_{2v}$, whereas the symmetry of [111]-oriented QWs belongs to the $C_{3v}$ point group. For [111]-oriented QWs, the HH states have the $\Gamma_5$ and $\Gamma_6$ representations and the LH states have the $\Gamma_4$ representation. The different representations in [111]-oriented QWs prohibit the HH-LH mixing, leading to the k-cubic Rashba SOC. The emergence of k-cubic Rashba SOC in [111]-oriented QWs and k-linear Rashba SOC in [001]-oriented QWs fully supports the postulation that the observed HH-LH mixing in [001]-oriented QWs arises from the local interface, although the global symmetry forbids it.

### TABLE I: Double point groups without interfaces and point groups of interfaces with corresponding irreducible representations of HH and LH states in different oriented QWs$^{54,59,60}$

| Orientation | [001] | [110] | [111] |
|-------------|-------|-------|-------|
| Point groups without interfaces | $D_{2d}$ | $C_{2v}$ | $C_{3v}$ |
| HH | $\Gamma_6$ | $\Gamma_5$ | $\Gamma_5, \Gamma_6$ |
| LH | $\Gamma_7$ | $\Gamma_5$ | $\Gamma_4$ |
| Point groups of interfaces | $C_{2v}$ | $C_{2v}$ | $C_{3v}$ |
| HH | $\Gamma_5$ | $\Gamma_5$ | $\Gamma_5, \Gamma_6$ |
| LH | $\Gamma_5$ | $\Gamma_5$ | $\Gamma_4$ |

### IV. DISCUSSION AND CONCLUSION

In experiments, one deduces the Rashba parameters $\alpha_R$ and $\gamma_R$ by measuring the spin relaxation length $l_{so}$ from magnetotransport measurements. This indirect measurement requires an analysis of weak localization and antilocalization involving the fitting of three quantities: the effective magnetic field induced by k-linear spin-orbit coupling $B_{SO1}$, the effective magnetic field induced by k-cubic spin-orbit coupling $B_{SO3}$ and the effective magnetic field for phase coherence $B_0$.$^{32,58,61}$ In this work, we directly obtain the Rashba parameters in QWs grown in different orientations by extracting our SEPM calculated band structure. Our work provides concrete guidance for experiments: (i). QWs in [110] crystalline orientation is the platform of the largest k-linear Rashba SOC; (ii). QWs in [111] crystalline orientation is the platform of the k-cubic Rashba SOC; (iii). QWs in [mmn] crystalline orientation also provide the k-linear Rashba SOC, but these Rashba parameters are much smaller than the [110] crystalline orientation and decrease with increasing the Miller index $n$. Experimentalists can select QWs grown in specific directions for k-linear or k-cubic, strong or weak Rashba SOC according to their concrete demands.

In conclusion, we systematically study the orientation-dependent k-linear Rashba SOC of 2DHGs in QWs and find the upper and lower bound in the [110] and [111] crystalline orientations, respectively. We reveal the intrinsic HH-LH mixing as the dominant factor to influence the Rashba SOC. We illustrate that only k-cubic Rashba SOC exists in [111]-oriented QWs, and further study the field- and size-dependencies of this k-cubic Rashba SOC. These findings improve the theoretical understanding of the Rashba SOC in 2DHGs of different oriented QWs and provide a strategic prediction for experiments related to the Rashba effect in QWs.
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