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Anisotropic refraction and valley-spin-dependent anomalous Klein tunneling in a 1T′-MoS_2-based p–n junction

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We investigate the transport properties of electron in a 1T′-MoS_2-based p–n junction. The anisotropic refraction of electron is found when the electron beam crosses the p–n junction, which brings the phenomenon of valley splitting without any external fields. Moreover, it is found that the valley-spin-dependent anomalous Klein tunneling, i.e., the perfect transmission exists at a nonzero incident angle of valley-spin-dependent electron, happens when the vertical electric field is equal to the critical electric field. These two peculiar properties arise from the same reason that the tilted band structure makes the directions of wavevector and velocity different. Our work designs a special valley splitter without any external fields and finds a new type of Klein tunneling.

Keywords: 1T′-MoS_2, anisotropic refraction, valley splitting, Klein tunneling

PACS: 73.22.Pr, 73.20.At, 78.67.–n **DOI:** 10.1088/1674-1056/ac46bf

1. Introduction

The discovery of two-dimensional transition metal dichalcogenides,[1] (TMDCs, the generalized formula MX_2 with M = Mo, W and X = S, Se, Te) provides a highly practical and prospective platform for studying energy storage,[2] next-generation electronics and photonics,[3,4] novel topological electronic devices,[5,6] and heterostructure.[7] TMDCs monolayer has three typical structures, i.e., 2H, 1T, and 1T′ structures.[6,8,9] Noticeably, 1T′-MX_2 was predicted to possess tilted Dirac band structure by first-principles calculations[6] and has been prepared in experiment,[10–13] which distinguishes from the band structure of 2H and 1T structures (untilted Dirac band structure). Generally, compared with an untilted system, the tilted system shows a wide range of extraordinary properties, such as anisotropic plasmons,[14] anisotropic optical conductivity,[15] anomalous Klein tunneling,[16–20] and anomalous Andreev reflection.[21] Therefore, the tilted Dirac band structure of 1T′-MX_2 also attracts researchers to find unusual physical properties, e.g., anisotropic longitudinal optical conductivities in 1T′-MoS_2 monolayer.[22] Here, we focus on the valley-dependent transport properties of electron in a 1T′-MoS_2-based p–n junction.

Electrons in some materials can occupy some separated low energy states called valley in the momentum space. The earliest concept of valley degree of freedom can trace back to 1970s.[23,24] At the beginning of 21th century, valley-dependent physical properties were discussed in some traditional materials such as silicon[25] and AlAs quantum wells.[26] The concept of valleytronics, being similar to charge-based electronics and spin-based spintronics, emerged in graphene based on the manipulation of valley degree of freedom.[27,28] After that, a variety of Dirac materials, e.g., silicene,[29] TMDCs monolayer,[30,31] and borophene,[32] were predicted to provide an important platform for realizing valleytronic devices such as valley filter,[27,33–35] valley valve,[36–38] and valley splitter.[39,40] The generation of valley polarization is a key factor for valleytronics applications. Traditionally, valley polarization is nonexistent in Dirac materials due to the valley degeneracy and hence the method of applying external fields, e.g., electric field, light illumination, and strain, is an efficient method to generate valley polarization.[41–47] In this paper, owing to the anisotropic refraction of electron, we find that the valley splitter can be realized in a 1T′-MoS_2-based n–p junction without any external fields.

In high energy physics, when a relativistic electron at the normal incidence crosses a potential barrier, the full transmission will happen regardless of the height and width of potential barrier, known as Klein tunneling.[48,49] In condensed state physics, Klein tunneling was firstly discussed in a graphene-based n–p–n junction,[50] which attracted tremendous interest in both theory and experiment.[51–54] Here the incident angle of electron is equal to zero when the Klein tunneling happens. However, the valley-dependent anomalous Klein tunneling, i.e., the full transmission at nonzero valley-dependent incident angle, was investigated in some anisotropic materials such as black phosphorus superlattices-based n–p–n junction,[16] Dirac–Weyl fermion systems,[17] 8-*Pmmn* borophene,[18,19] and borophane recently.[29] In this study, we find a valley-spin-dependent anomalous Klein tunneling in a 1T′-MoS_2-based p–

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n junction.

The paper is organized as follows. We firstly give the model and basic formalism. Then, the numerical results and theoretical analysis are presented and discussed. Finally, the main results of this work are summarized.

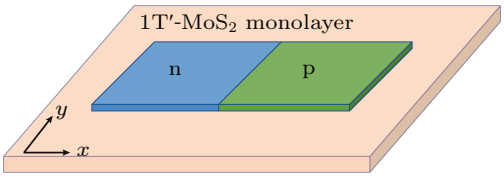


Fig. 1. Schematic diagrams for 1T′-MoS_2-based p–n junction.

2. Models and methods

The uniform Hamiltonian for 1T′-MoS_2-based p–n junction shown in Fig. 1 reads[6,22]

$$\begin{aligned} H_\eta &= \hbar k_x v_x \sigma_y + \hbar k_y [v_y \sigma_x - \eta (v_- \sigma_0 + v_+ \sigma_z)] \\ &\quad + \lambda_{\rm so} \sigma_x (\eta - \alpha\sigma) + V\sigma_0. \end{aligned} \tag{1}$$

Here, the spin–orbit coupling-induced gap $\lambda_{\rm so} = 42$ meV and the velocities $v_x = 0.387 v_{\rm F}$, $v_y = 0.046 v_{\rm F}$, $v_+ = 0.721 v_{\rm F}$, and $v_- = 0.286 v_{\rm F}$ with $v_{\rm F} = 10^6$ m/s; $\eta = +(-)$ represents $\Lambda(-\Lambda)$ valley index;[6,22] σ is the spin index; $\sigma_{x,y,z}$ and σ_0 denote the Pauli matrix and unit matrix, respectively; α is equal to $|E_z/E_{\rm c}|$ with the vertical electric field E_z and the critical electric field $E_{\rm c}$ for topological phase transition.[6] Potential barrier $V = V_0$ (0) in p (n) region can be adjusted by gate voltage or doping. The energy dispersion of Eq. (1) is

$$E^{\pm}_{\eta\sigma} = V - \eta\hbar k_y v_- \pm \sqrt{M}, \tag{2}$$

where $M = (\hbar k_y v_+)^2 + (\hbar k_x v_x)^2 + [\hbar k_y v_y + \lambda_{\rm so}(\eta - \alpha\sigma)]^2$, $+$ $(-)$ denotes conduction (valence) band, and parameter v_- makes the band structure tilted along k_y direction.

The wavefunctions in left and right regions are

$$\begin{aligned} \Psi_{\rm L} &= \psi^{\rm i}_{\rm L} + r\psi^{\rm r}_{\rm L}, \\ \Psi_{\rm R} &= t\psi^{\rm t}_{\rm R}, \end{aligned} \tag{3}$$

where r is the reflection coefficient and t is the transmission coefficient. The incident, reflected, and transmitted wavefunctions in each region are

$$\begin{aligned} \psi^{\rm i(r)}_{\rm L} &= \left(1, \frac{{\rm i}\hbar v_x k^{\rm i(r)}_x + \hbar v_y k_y + \Delta}{\varepsilon + \eta\hbar k_y (v_- - v_+)}\right)^{\rm T} {\rm e}^{{\rm i}(k^{\rm i(r)}_x x + k_y y)}, \\ \psi^{\rm t}_{\rm R} &= \left(1, \frac{{\rm i}\hbar v_x k^{\rm t}_x + \hbar v_y k_y + \Delta}{\varepsilon + \eta\hbar k_y (v_- - v_+) - V_0}\right)^{\rm T} {\rm e}^{{\rm i}(k^{\rm t}_x x + k_y y)}, \end{aligned} \tag{4}$$

where Δ is equal to $\lambda_{\rm so}(\eta - \alpha\sigma)$. T represents the transformation of matrix, ε is the incident energy of electron. In the process of calculation, we consider the incident electron from conduction band and therefore the magnitudes of $k^{\rm i(r)}_x$ and k_y meet $\varepsilon = E^+_{\eta\sigma}$ while the magnitudes of $k^{\rm t}_x$ and k_y meet $\varepsilon = E^-_{\eta\sigma}$. Then, the matching condition for the wavefunctions at the interface of 1T′-MoS_2-based p–n junction is given as

$$\Psi_{\rm L}(0) = \Psi_{\rm R}(0), \tag{5}$$

and the corresponding valley-spin-dependent reflection coefficient is written as

$$r_{\eta\sigma} = \frac{B_{\rm t} - A_{\rm i}}{A_{\rm r} - B_{\rm t}}, \tag{6}$$

where

$$\begin{aligned} A_{\rm i(r)} &= \frac{{\rm i}\hbar v_x k^{\rm i(r)}_x + \hbar v_y k_y + \Delta}{\varepsilon + \eta\hbar k_y (v_- - v_+)}, \\ B_{\rm t} &= \frac{{\rm i}\hbar v_x k^{\rm t}_x + \hbar v_y k_y + \Delta}{\varepsilon + \eta\hbar k_y (v_- - v_+) - V_0}. \end{aligned} \tag{7}$$

The valley-spin-dependent transmission probability across p–n junction is written as $T_{\eta\sigma} = 1 - r^*_{\eta\sigma} r_{\eta\sigma}$.

3. Results and discussion

3.1. Anisotropic refraction

The velocity components of electron are calculated by formula $\boldsymbol{u} = \frac{1}{\hbar}\nabla_{\boldsymbol{k}} E$,

$$\begin{aligned} u^{\pm}_x &= \frac{\partial E^{\pm}_{\eta\sigma}}{\hbar \partial k_x} = \pm \frac{\hbar v_x^2 k_x}{\sqrt{M}}, \\ u^{\pm}_y &= \frac{\partial E^{\pm}_{\eta\sigma}}{\hbar \partial k_y} = -\eta v_- \pm \frac{\hbar v_+^2 k_y + (\hbar v_y k_y + \Delta) v_y}{\sqrt{M}}. \end{aligned} \tag{8}$$

We consider the incident (transmitted) electron from conduction (valence) in n (p) region. Then the valley-spin-dependent incident angle of electron in n region and the refracted angle of electron in p region are defined as

$$\varphi^{\eta\sigma}_{\rm i} = \arctan \frac{u^+_y}{u^+_x}\bigg|_{k_x = k^{\rm i}_x}, \quad \varphi^{\eta\sigma}_{\rm t} = \arctan \frac{u^-_y}{u^-_x}\bigg|_{k_x = k^{\rm t}_x}. \tag{9}$$

The valley-spin-dependent refractive index of electron is defined as

$$n_{\eta\sigma} = \frac{\sin \varphi^{\eta\sigma}_{\rm i}}{\sin \varphi^{\eta\sigma}_{\rm t}}. \tag{10}$$

The valley-spin-dependent refractive index as a function of incident angle are given in Fig. 2 in the different values of α. The signs of refractive index for two valleys are opposite completely in Fig. 2 regardless of the value of α. Although the spin-dependent refractive index in one valley can be tuned by the external electric field, the signs of refractive index for spin-up and spin-down in one valley are the same, as shown in Figs. 2(b)–2(c). This unusual valley-spin-dependent refractive index brings exotic relations between incident angle and transmitted angle, as shown in Fig. 3, in which the valley-spin-dependent transmitted angle as a function of incident angle is given in the different values of α. In Fig. 3(a) with $\alpha = 0$, the

spin is degeneracy and the sign of transmitted angle is negative (positive) for Λ $(-\Lambda)$ valley. In Figs. 3(b)–3(c) with the nonzero α, the valley-spin-dependent transmitted angles are shown. Although the spin-dependent transmitted angles in one valley are different, their signs are the same in one valley. These results in Fig. 3 are consistent with those in Fig. 2 and will bring a potential application for valley splitting without any external fields.

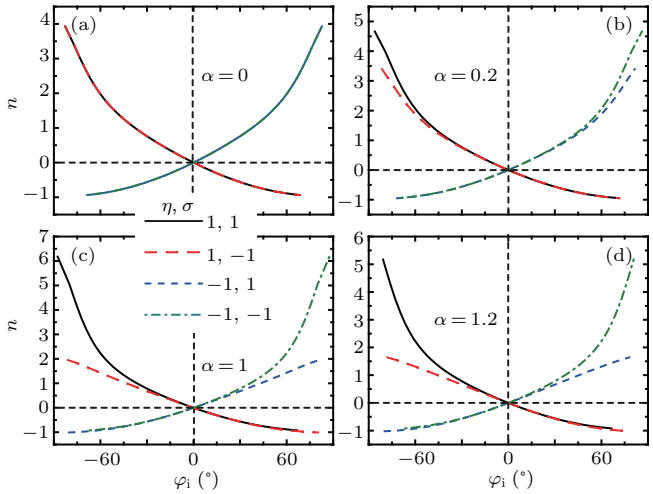


Fig. 2. Incident angle-dependent refractive index with $\varepsilon = 0.1$ eV and $V_0 = 0.3$ eV in the different values of α.

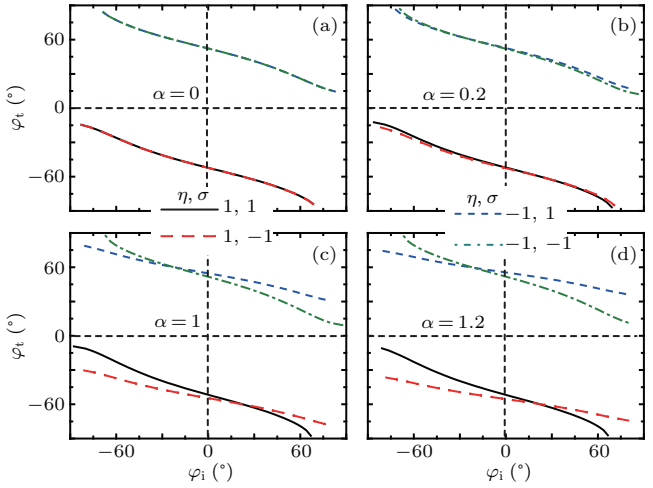


Fig. 3. Incident angle-dependent transmitted angle with $\varepsilon = 0.1$ eV and $V_0 = 0.3$ eV in the different values of α.

Why does the valley splitting happen in a 1T′-MoS_2-based p–n junction? Let us pay attention to Eq. (8). We assume physical parameter $v_- = 0$, then the valley-spin-dependent incident angle of electron in n region and the refracted angle of electron in p region can be rewritten as

$$\varphi_i^{\eta\sigma} = \arctan \left. \frac{\hbar v_+^2 k_y + (\hbar v_y k_y + \Delta) v_y}{\hbar v_x^2 k_x} \right|_{k_x = k_x^i},$$
$$\varphi_t^{\eta\sigma} = \arctan \left. \frac{\hbar v_+^2 k_y + (\hbar v_y k_y + \Delta) v_y}{\hbar v_x^2 k_x} \right|_{k_x = k_x^t}. \quad (11)$$

The signs of $\varphi_i^{\eta\sigma}$ and $\varphi_t^{\eta\sigma}$ are opposite completely due to the conversion of transverse wavevector k_y and the opposite signs of k_x^i and k_x^t. This analytical result is consistent with the numerical result in Fig. 4, in which the signs of $\varphi_i^{\eta\sigma}$ and $\varphi_t^{\eta\sigma}$ are opposite regardless of the value of α. Therefore, the presence of parameter v_-, which makes the band structure of 1T′-MoS_2 tilted, plays a key role in realizing valley splitting.

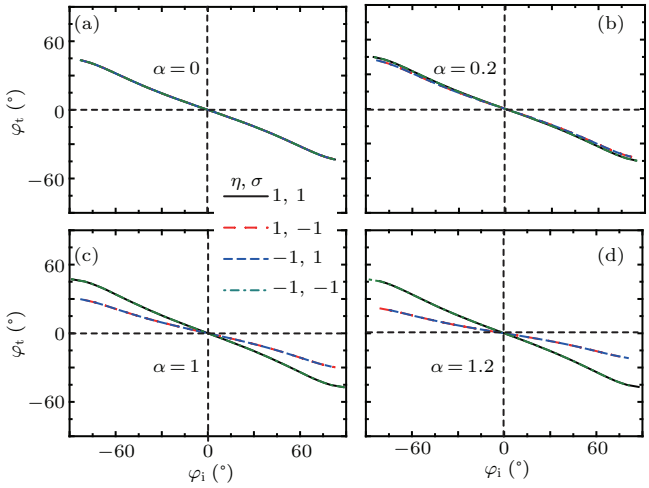


Fig. 4. Incident angle-dependent transmitted angle with $\varepsilon = 0.1$ eV, $v_- = 0$, and $V_0 = 0.3$ eV in the different values of α.

3.2. Valley-dependent anomalous Klein tunneling

Using Heisenberg's equation of motion, we can write the velocity operator of electron along x direction as $\hat{u}_x = \frac{1}{i\hbar}[x, H_\eta] = v_x \sigma_y$, and then its time evolution is given as

$$\dot{\hat{u}}_{x'e} = \frac{1}{i\hbar}[\hat{u}_x, H_\eta] = -2k_y v_x (v_y \sigma_z + v_+ \sigma_x) - \frac{2\Delta v_x \sigma_z}{\hbar}, \quad (12)$$

in which $\Delta = \lambda_{so}(\eta - \alpha\sigma)$. We give the incident angle of Klein tunneling when $k_y = 0$ and $\Delta = 0$,

$$\varphi_{ei} = \arctan\left(-\frac{\eta v_-}{v_x}\right). \quad (13)$$

It is easy to obtain $\varphi_{ei} \approx -(+)36.5°$ for $\eta = \sigma = 1(-1)$ regardless of the value of V_0, which is the same as the numerical results in Figs. 5 and 6. Interestingly, the angle of Klein tunneling is dependent on the valley and spin simultaneously, which is different from the valley-spin-independent Klein tunneling and valley-dependent Klein tunneling.

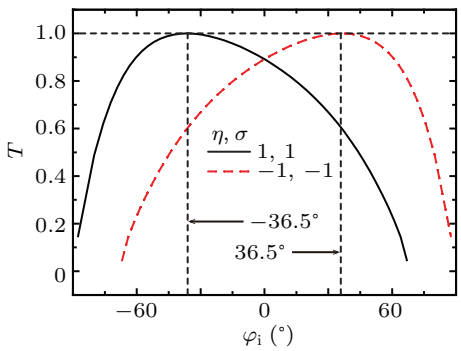


Fig. 5. Incident angle-dependent transmission with $\varepsilon = 0.1$ eV, $\alpha = 1$, and $V_0 = 0.3$ eV.

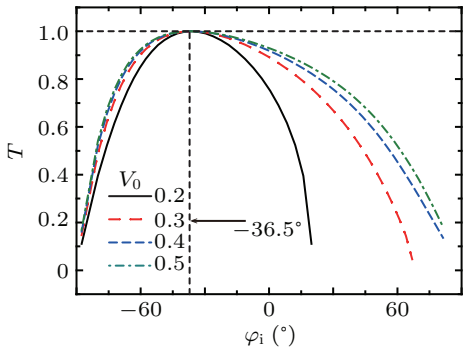


Fig. 6. Incident angle-dependent transmission with $\varepsilon = 0.1$ eV, $\eta = 1$, $\sigma = 1$, and $\alpha = 1$ for different values of V_0.

4. Conclusion

We now give some discussions on experimental realization of our theoretical proposal. In experiment, the preparation of 1T′-MoS2 was reported in Ref. [55]. The 1T′-MoS2 based p–n junction can be realized by doping. The similar setup has been successfully realized for graphene.[52,56,57] A beam of electrons splits into two beams, which is the signature of valley splitting. The nonzero incident angle of electron for full transmission is the signature of anomalous Klein tunneling.

In conclusion, the transport properties of electron is investigated analytically in a 1T′-MoS_2-based p–n junction. The anisotropic refraction consisting of positive and negative refractions is found, which leads to the valley splitting without any external fields. Interestingly, the nonzero incident angle of valley-spin-dependent anomalous Klein tunneling happens. These two peculiar properties come from the same fact that the tilted band structure makes the directions of wavevector and velocity different. Our work designs an special valley splitter without any external fields and provides an insight into the understanding of the Klein tunneling.

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