Gate-controlled valley transport and Goos–Hänchen effect in monolayer WS$_2$

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Abstract

Based on a Dirac-like Hamiltonian and coherent scattering formalism, we study the spin-valley transport and Goos–Hänchen-like (GHL) effect of transmitted and reflected electrons in a gated monolayer WS$_2$. Our results show that the lateral shift of spin-polarized electrons is strongly dependent on the width of the gated region and can be positive or negative in both Klein tunneling and classical motion regimes. The absolute values of the lateral displacements at resonance positions can be considerably enhanced when the incident angle of electrons is close to the critical angle. In contrast to the time reversal symmetry for the transmitted electrons, the GHL shift of the reflected beams is not invariant under simultaneous interchange of spins and valleys, indicating the lack of spin-valley symmetry induced by the tunable potential barrier on the WS$_2$ monolayer. Our findings provide evidence for electrical control of valley filtering and valley beam splitting by tuning the incident angle of electrons in nanoelectronic devices based on monolayer transition metal dichalcogenides.

Keywords: valley polarization, lateral shift, layered transition metal dichalcogenides, spin-valley transport

(Some figures may appear in colour only in the online journal)

1. Introduction

Two-dimensional (2D) materials such as monolayers of transition metal dichalcogenides (TMDs) have attracted considerable attention due to their fascinating physical properties. In contrast to the zero-gap graphene, they are direct gap semiconductors with sizable bandgaps in the visible spectrum which make them promising materials in electronic and optoelectronic applications such as field-effect transistors and light-emitting diodes [1, 2]. The layered TMDs such as MoS$_2$ and WS$_2$ monolayers possess strong spin–orbit coupling due to the $d$ orbitals of heavy metal atoms, causing a large spin splitting (~440 meV in WS$_2$ monolayers) in the valence bands [3, 4]. Moreover, the absence of inversion symmetry in the crystal structure of these materials allows valley polarization of carriers by optically exciting electrons with a circularly polarized light [5–10]. The valleys occur at the non-equivalent K and K' points in the hexagonal Brillouin zone of TMD monolayers [5]. Manipulating both the spin and valley degree of freedoms in such monolayers makes it possible to design a new generation of nanoelectronic devices for quantum computing [5, 7, 8, 10].

It was demonstrated that the electrons and holes at the band edges of MoS$_2$ monolayers and other layered group-VI dichalcogenides can be well described by massive Dirac fermions with strong spin-valley coupling [5]. On the other hand, due to the similarities between propagation of Dirac fermions and propagation of electromagnetic waves in dielectrics, many optical phenomena such as Brewster angles [11], collimation [12], Bragg reflection, electronic lenses [13, 14] and Goos–Hänchen (GH) shift [15, 16] have been found in single-layer graphene. Among them, the GH effect refers to a lateral displacement of a light beam when it is totally reflected from a dielectric interface. In the past several years, most studies on the electronic GH shift have been devoted to graphene-based nanostructures such as graphene p-n junctions [16], strained graphene [11, 17], graphene with electric and magnetic barriers [18, 19], and valley [17] and spin [20] beam splitters in...
graphene. Recently, the GH effect of electrons has also been studied in silicene [21] and a p-n-p junction of MoS$_2$ monolayer [22]. It was found that the GH shift of Dirac fermions, which has a magnitude of the order of Fermi wavelength [23, 24], can be amplified by multiple total internal reflections [22, 24]. Moreover, the lateral shifts of Dirac fermions in transmission through semiconductor barriers [25], graphene single barrier [23], double barrier [26], and multiple barrier structures [27] have also been reported. Such displacements, called Goos–Hänchen like (GHL) shifts, occur in the partial reflection regime and can be intensified by the transmission resonances (Fabry–Perot resonances). However, it is still a challenging problem to experimentally observe the GH or GHL shifts of electrons due to the small size of the shifts and also the difficulty in producing a well-collimated electron beam [24]. On the other hand, to design a beam splitter and also the difficulty in producing a well-collimated electron beam [24], and the critical angle for total reflection can be obtained by setting $V_g(0)d < \lambda_F$ and $V_g(d) > \lambda_F$. According to equation (1), the dispersion relation in the gated region II is given by

$$\mathcal{H} = a\tau k_x \hat{\sigma}_x + k_y \hat{\sigma}_y + \frac{\Delta}{2} \hat{\sigma}_z - \lambda \tau \hat{\sigma}_z - \frac{1}{2} \hat{\sigma}_z + V_G \Theta(x) \Theta(d - x),$$

where $a$ is the lattice constant, $\tau$ is the effective hopping integral, and $\tau = 1(-1)$ is the valley index corresponding to $K (K')$ point. $k_{x,y,z}$ denote the components of an electron wave vector measured from $K$ and $K'$, $\sigma_{x,y,z}$ are the Pauli matrices spanning the conduction and valence states in the two valleys, $\Delta$ is the band gap between valence and conduction bands, and $2\lambda$ is the spin-splitting at the valence band maximum due to the spin–orbit interaction. $\hat{\sigma}_z$ is the $z$ component of Pauli matrix for electron spin and $\Theta(x)$ is the Heaviside step function. According to equation (1), the dispersion relation in the gated region II is given by

$$2(E - 2V_g - \tau \sigma_z \lambda)^2 - (\Delta - \tau \sigma_z \lambda)^2 = (2ak')^2,$$

where $k' = \sqrt{k_x^2 + k_y^2}$ and $\sigma_z = \pm 1$ which stands for spin up ($\uparrow$) and spin down ($\downarrow$). In the regions I and III, however, the relation can be obtained by setting $V_G = 0$ and replacing $k'$ with $k = \sqrt{k_x^2 + k_y^2}$.

Now we consider the propagation of spin-polarized electrons in the WS$_2$ junction which can be scattered by the potential barrier, induced by the gate voltage $V_G$. It is assumed that the spin-polarized electrons are injected by a magnetic contact, such as a ferromagnetic semiconductor [10, 28], into the

Figure 1. Schematic model for the gated monolayer WS$_2$ in which the gated region acts as a tunable potential barrier. (b) Energy profile of the model shown in (a) for an incident electron with spin $\sigma_z(\hat{\sigma}_z)$ in valley $K$ ($K'$) and a typical value $V_G < \Delta, E_c$ and $E_v$ denote the energy of conduction band minimum and valence band maximum, respectively. The red and blue lines show the spin-dependent energy levels at the top of the valence band, due to the spin–orbit coupling. Note that the spin splitting at the different valleys are opposite due to the time-reversal symmetry.

2. Model and formalism

To explore the effect of GHL shift in a TMD monolayer with a tunable potential barrier, we consider a single-layer of WS$_2$ in $x - y$ plane and apply a top gate voltage to the region II ($0 < x < d$), while the regions I ($x < 0$) and III ($x > d$) are kept at a zero electrostatic potential, as shown in figure 1. The top gate voltage induces a potential barrier with the height $V_G$ (figure 1(b)), and turn the system into a n-p-n WS$_2$ junction. This means that the electronic transport through the junction can be strongly affected by the gate. We emphasize here that the gate voltage in the proposed model is only utilized to shift the energy levels but not to modulate the energy gap. In this normal/gated/normal WS$_2$ junction, the low-energy electrons near valleys $K$ and $K'$ can be described by the Dirac-like Hamiltonian [5]

$$\mathcal{H} = a\tau k_x \hat{\sigma}_x + k_y \hat{\sigma}_y + \frac{\Delta}{2} \hat{\sigma}_z - \lambda \tau \hat{\sigma}_z - \frac{1}{2} \hat{\sigma}_z + V_G \Theta(x) \Theta(d - x),$$
left normal region. For simplicity, the source of spin injection is not included in the model. We further assume that the dimension of the monolayer along the y-axis is infinitely long. Therefore, due to the translational invariance in the y direction, $k_y$ is conserved, and the electron wave function in each region can be described as

$$
\psi_1 = \frac{1}{B_1} \left( A_1 e^{-i(k_x x + k_y y)} + r_x^{F_{1}} \left( -A_1 e^{-i(k_x x + k_y y)} \right) \right),
$$

$$
\psi_2 = \frac{\alpha}{B_2} \left( A_2 e^{-i(k'_x x + k'_y y)} + r_x^{F_{2}} \left( -A_2 e^{-i(k'_x x + k'_y y)} \right) \right),
$$

and

$$
\psi_3 = \frac{A_3}{B_3} e^{i(k_x x + k_y y)},
$$

where $\varphi = \tan^{-1}(k_y/k_x)$ is the incident angle of electrons on the barrier, $r_x^{F_{1,2}}$ is the reflection amplitude, $\varphi' = \tan^{-1}(k'_y/k'_x)$ is the angle of refraction, and $t_x$ is the transmission amplitude of electrons. The coefficients $A_i, B_i (i=1,2,3)$ in equations (3)-(5) are expressed as $A_1 = A_2 = E - \varphi_x \lambda + \Delta \Delta_1, A_2 = A_1 - V_G, B_1 = B_2 = \sqrt{\lambda_1^2 + (at)^2},$ and $B_2 = \sqrt{\lambda_2^2 + (at')^2}.$

The total internal reflection of electrons occurs if the incident electron waves strike the potential barrier at a critical angle $\varphi_c$ which is given by

$$
\varphi_c = \arcsin \sqrt{\frac{2(1 - V_G - \varphi_x \lambda)^2 - (\Delta - \varphi_x \lambda)^2}{(1 - \varphi_x \lambda)^2 - (\Delta - \varphi_x \lambda)^2}}.
$$

When the angle of incidence $\varphi$ is greater than the critical angle, the electron wave vector in the electrostatic barrier, $k'_y = \sqrt{k^2 - k_y^2}$, becomes imaginary which indicates an evanescent wave in the gated region, and hence, the electron beam will experience a total reflection from the electrostatic barrier. In the case of $\varphi < \varphi_c$, however, the electron wave is partially reflected and partially transmitted. The coefficients $r_x^{F_{1,2}}, \alpha, \beta,$ and $t_x^{F}$ can be obtained by applying the continuity of the wave functions at the two interfaces, $x = 0$ and $x = d$ shown in figure 1. The transmission $t_x^{F}$ and reflection $r_x^{F_{1,2}}$ coefficients for the electron waves are expressed as

$$
t_x^{F} = \frac{2s t_x^{F}}{2s t_x^{F}} \cos \varphi \cos \varphi' e^{-i(k'd)}.
$$

$$
r_x^{F_{1,2}} = \frac{-2s t_x^{F}}{2s t_x^{F}} \cos \varphi \cos \varphi'(k'd) - iD.
$$

where $D = [(1 + t_x^{F}) - 2s t_x^{F} \sin \varphi' \sin \varphi' \sin(k'd)]. F_1 = A_2/A_1, F_2 = (E - V_G - \Delta^2/2)/(E - \Delta^2), s = \text{sgn}(A_1), \text{and } s' = \text{sgn}(A_2).$

To study the GHL effect, we consider an incident electron in the form of a Gaussian wave packet of the width $\Delta k_y$ and energy $E$.

$$
\psi_{in}(x,y) = \int_{-\infty}^{+\infty} dk_y f(k_y-k_y) \frac{1}{B_1} \left( A_1 e^{-i(k_x x + k_y y)} \right),
$$

where the Gaussian $f(k_y-k_y) = e^{-i(k_y-k_y)^2/2k_x^2}$ shows the angular distribution of electron beam around the central incidence angle $\varphi_0 = \arcsin(k_y/k).$ Therefore, the transmitted electron beam can be given as

$$
\psi_{tr}(x,y) = \int_{-\infty}^{+\infty} dk_y \frac{1}{B_1} \left( A_1 e^{-i(k_x x + k_y y)} \right) e^{i(k_y-k_y)2k_x^2},
$$

where $\varphi_0 = \arcsin(k_y/k).$ Here, the dot denotes the derivative with respect to $k$. Therefore, the two components of $\psi_{in}$ represent two Gaussians of the same width, centered at the two different mean coordinates $\bar{y}^+_{in}$ and $\bar{y}^-_{in}$ along the y-axis.

Using a similar analysis, the transmitted electron beam can be expressed as

$$
\psi_{tr}(x,y) = \frac{\sqrt{2\pi} \Delta k_y}{B_1} e^{i(k_y-y)\lambda + \Delta \lambda_1^2/2} \left( \frac{A_1}{\text{sgn}(A_1)} e^{-i(k_x x + k_y y)} \right).
$$

where $\bar{y}^+_{tr} = -\hat{k}_x(k_y)k_x - \Phi_{in}^+(k_y)$ and $\bar{y}^-_{tr} = -\hat{k}_x(k_y)k_x - \Phi_{in}^-(k_y).$ Note that $\Phi_{in}^+$ in equation (12) and in the mean coordinates $\bar{y}^+_{tr}$ denotes the phase of transmission coefficient $t_x^{F}$. Accordingly, the GHL shifts of the upper and lower components of the transmitted electrons are given by

$$
\sigma_{\pm} = \bar{y}^+_{\pm} - \bar{y}^-_{\pm} = -\Phi_{in}^\pm (k_y) d.
$$

Since the two components have equal shift values, the average GHL shift of the transmitted beam can be expressed as

$$
\sigma_{tr} = -\Phi_{in}^+ (k_y) - \hat{k}_x(k_y) d.
$$

Applying similar considerations to the lateral shift of the reflected beam, we find that $\sigma_x = -\Phi_{in}^+ (k_y) \hat{k}_x$. By considering the probability of upper and lower components of the beams, the average shift of reflected electrons will be

$$$
\sigma_{\pm} = \bar{y}^+_{\pm} - \bar{y}^-_{\pm} = -\Phi_{in}^\pm (k_y) d.
$$

Since the two components have equal shift values, the average GHL shift of the reflected beam can be expressed as

$$$
\sigma_{tr} = -\Phi_{in}^+ (k_y) - \hat{k}_x(k_y) d.
$$
In the case of a transmitted beam, we need to calculate \( \Phi_{\tau+ \sigma} \) from equation (7), and substitute into equation (14). Thus, the lateral electrostatic potential can be obtained by

\[
\sigma_{\tau+ \sigma}^T = \frac{1}{B_{1}^2} \left[ A_1^2 \alpha_s + (ak)^2 \alpha_s \right] + \frac{2\tau \alpha_s^2 k^2}{B_{1}^2} \varphi(k_{\alpha_s}). \tag{15}
\]

where \( k_{\alpha_s}^2 = -ss'kk' + 2k_0^2 \) and \( \gamma = \sqrt{F_1/F_2}(1 + F_1/F_2) \).

On the other hand, by computing \( \Phi_{\tau+ \sigma} \) from equation (8) and substituting into equation (15), the GHL shift for the reflected wave can be written as

\[
\sigma_{\tau+ \sigma}^R = \sigma_{\tau+ \sigma}^T + \frac{2\tau}{k_x} \left[ C_1 + C_2 = C_3 \right] \left( \frac{B_{1}^2(1 + C_0)}{B_{1}^2} \right), \tag{17}
\]

where

\[
C_0 = \left[ \frac{F_1}{F_2} + \frac{k_0^2}{k'^2} - 2(k_0^2 - k'^2) \right] \frac{F_1}{F_2} - 4ss' k_0^2 kk' (1 + F_1/F_2) \sqrt{\frac{F_1}{F_2}}, \tag{18}
\]

\[
C_1 = a^2r^2k^2 - A_1^2 \frac{F_3}{F_2} + (a^2r^2k^2 - A_1^2) \left[ \frac{2k_0^2}{k'^2} + \frac{k_0^2 - k'^2}{k'^2} \right] \frac{F_1}{F_2} \tag{19}
\]

\[
C_2 = ss' [k_0^2(a^2r^2k^2 + A_1^2) - k_0^2(2a^2r^2k^2 - 3A_1^2)] \frac{1}{kk'} \sqrt{\frac{F_3}{F_2}}, \tag{20}
\]

\[
C_3 = ss' [k_0^2(a^2r^2k^2 + A_1^2) + k_0^2(3a^2r^2k^2 - A_1^2)] \frac{1}{kk'} \sqrt{\frac{F_1}{F_2}}. \tag{21}
\]

It is important to note that the GHL shift for the transmitted wave is dependent on the product of \( s \times \tau \), as can be seen from the expressions, \( F_1, F_2, s, s' \), and equation (2). In other words, the GHL shift for the transmitted wave has a \( s \times \tau \) (spin-valley) symmetry [29], whereas such a symmetry cannot be seen in the GHL shift of the reflected wave, due to the presence of the second term in equation (17). In fact, the reflected beam is not only dependent on the product of \( \tau \) and \( s \), but also on the valley index \( \tau \), separately, indicating that the reflected electron does not remain invariant under the simultaneous interchange of spins and valleys in this system.

3. Limiting cases in GHL shift

Now we consider some limiting cases to show how the present formalism is also able to reproduce the analytic results of previous studies in MoS\(_2\) and graphene single interfaces [16, 22], and also the graphene barrier [23].

3.1. Single interface on TMD monolayers

As already mentioned, for incident angles greater than the critical angle, \( \varphi > \varphi_c \), the wave vector \( k_x' \) becomes imaginary and hence, the total reflection occurs. In such a case, equation (17) which is given for \( \varphi < \varphi_c \) is valid for \( \varphi > \varphi_c \), provided that we make the substitution \( k_x' \rightarrow ik \). After this substitution and taking the limit \( d \rightarrow \infty \), the second term in equation (17) does not change, but the first term becomes

\[
\frac{[8k_0^2k^2 + 2k_0^2(k^2 - k_x^2)] tan \varphi}{k(4k_0^2k^2 + 2k_0^2)}, \tag{22}
\]

Therefore, the GH shift of the totally reflected beam from a step potential (single interface) applied on a monolayer of TMD, can be easily calculated by replacing the first term of equation (17) by (22).

In [22], the probabilities of upper and lower components of the reflected electrons have not been included in the calculations and the average GH shift was simply computed by \( \sigma_{\tau+ \sigma}^R = \frac{1}{2} (\sigma_+ + \sigma_-) \). On this basis, the second term in equation (17) becomes \( \frac{1}{k_x} \left[ 1 - \frac{F_1}{F_2} - 2ss' \frac{F_1}{F_2} (1 + F_1/F_2) \right] \), and finally the GH shift of the totally reflected beam can be simplified as

\[
\sigma_{\tau+ \sigma}^R = \frac{\frac{1}{k_x} [(\tau \kappa + k_x)^2 - k_0^2(k_x^2 - k_x' \bar{k}) + \frac{2\kappa \kappa'}{\tau \kappa} \kappa' \sin \varphi]}{\frac{1}{k_x} [(\tau \kappa + k_x)^2 + k_0^2(k_x^2 - k_x' \bar{k}) + \frac{2\kappa \kappa'}{\tau \kappa} \kappa' \sin \varphi]}, \tag{23}
\]

This equation is exactly the same as equation (8) given in [22] for MoS\(_2\) monolayers.

3.2. Graphene barrier

By setting \( \lambda = 0 \) and \( \Delta = 0 \) in equations (1), (16) and (17), the Hamiltonian of gapless graphene with a tunable potential barrier and the corresponding GHL shifts for transmitted and reflected beams can be obtained, respectively [23]. In this regard, the lateral shifts of the reflected and transmitted electron beams in graphene are the same and expressed as

\[
\sigma_{\tau+ \sigma}^R = \sigma_{\tau+ \sigma}^T \
= \frac{(2 + \frac{k_0^2}{k'^2} + \frac{k_0^2}{k'^2} \frac{sin(2kd')}{2kd'} - \frac{k_0^2}{k'^2}) \sin(2kd')}{cos^2(k_d') + \frac{k_0^2}{k'^2} \sin^2(k_d')}, \tag{24}
\]

where \( k_0'^2 = -ss'kk' + k_0^2 \). Note that in the case of \( \lambda = 0 \) and \( \Delta \neq 0 \) (gapped graphene), we obtain \( \sigma_{\tau+ \sigma} = \sigma_{\tau+ \sigma} \).

Equation (24) at \( ss' = \pm 1 \) is the same as equations (11) and (19) in [23], respectively. Moreover, in the case of \( ss' = -1 \), substituting \( k_x' \rightarrow ik \) for \( \varphi > \varphi_c \) into equation (24), and taking the limit \( d \rightarrow \infty \), one can obtain after some calculation

\[
\sigma = \frac{k_0^2 - kk'}{skk'}, \tag{25}
\]

Finally, using equation (2), we obtain

\[
\sigma = \frac{\sin^2 \varphi + 1 - V_d/E}{k \sin \varphi \cos \varphi}, \tag{26}
\]
This equation describes the GH shift of electrons in a total reflection from a step potential (single interface) on graphene. It is interesting to note that this expression is exactly the same as equation (11) given in [16]. Therefore, our present formalism in limiting cases is able to reproduce the previous results of GH shifts for single interfaces on graphene4 and TMD monolayers [22], and also GHL shift on graphene barrier [23].

4. Results and discussion

We present our numerical results for gated monolayer WS2 as a family member of layered TMD materials, using the parameters $t = 1.37$ eV, $\Delta = 1.79$ eV, $2\lambda = 0.43$ eV, and $a = 3.197$ Å [5]. From the dispersion relation, equation (2), the energy regions for electrons in propagating mode are given by $\frac{\Delta}{2} < E < V_G - \frac{\Delta}{2} + \tau_x \lambda$ and $E > V_G + \frac{\Delta}{2}$ associated with the Klein tunneling effect [23, 30–32] ($ss' = -1$) and the classical motion ($ss' = 1$), respectively. In both regimes, transmission probability, $T = |t'_{sz}|^2$, and lateral shift $\sigma_{tr, sz}$ of electrons with an energy value $E$ and a given $V_G$, are strongly dependent on the width $d$ of the gated region. Therefore, to compare these quantities in the two energy regions, we show in figure 2 the transmission probabilities and the GHL shifts of a transmitted electron beam with spin up ($s_z = 1$) through the gated monolayer, as the barrier width $d$ (normalized by $k'_x$) is increased.

At the resonance conditions $k'_d = n\pi (n = 0, \pm 1, \pm 2, \ldots)$, the potential barrier in both energy regions becomes fully transparent, $T = 1$, and the maximum absolute values of the lateral shifts are given by

$$\sigma_{tr, sz}^{K, K'} = \frac{k'_d \tan \varphi}{2k_x^2}. \quad (27)$$

Figure 2. Dependence of transmission probability and GHL shift of the transmitted electrons with $s_z = 1$ on the width $d$ of the gated region in ((a) and (b)) Klein tunneling and ((c) and (d)) classical motion, where $V_G = 3$ eV. The other parameters are: ((a) and (b)) $E = 1.75$ eV, $\varphi = 19.5^\circ$, and $\varphi_s = 50.10^\circ$ in K-valley, $\varphi_s = 20.5^\circ$ in K$'$-valley, ((c) and (d)) $E = 5.0$ eV, $\varphi = 20.5^\circ$, and $\varphi_s = 20.88^\circ$ in K-valley, $\varphi_s = 21.73^\circ$ in K$'$-valley. Note that $d$ is normalized with $k'_x$.

Note that only the first three maxima are shown in figures 2(b) and (d). In the Klein tunneling regime (figures 2(a) and (b)), the transmission probabilities and the lateral shifts are strongly dependent on the valleys K and K', whereas such a valley-dependent transport is weaker in the classical motion as shown in figures 2(c) and (d). Although the angle of incidence is closer to the critical angles in the classical regime compared to the Klein tunneling regime, the GHL effect in the Klein tunneling can more significantly separate the K and K' valley electron beams compared to the classical motion. For instance, the difference between the two lateral displacements at the third maximum absolute value is $\sim 1065$ nm in the Klein tunneling, while it is $\sim 227$ nm in the classical regime.

From equation (16), it is clear that the lateral shift is dependent on the angle of incidence. Moreover, $k'_x$ is zero at

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4 Due to a mistake in a minus sign, the authors of [23] could not obtain equation (11) in [16].
critical angle $\varphi_c$. Therefore, at incident angles $\varphi$ close to $\varphi_c$, the maximum absolute values of the shifts given by equation (27), can increase rapidly so that the spatial separation between $K$ and $K'$ electron waves in both regimes can exceed the width of incident beam. It should be mentioned that due to the presence of $s_z \cdot \tau$ symmetry in equation (16), the results given in figure 2 with $s_z = +1$ and $\tau = -1$ ($\tau = +1$) are the same as those with $s_z = -1$ and $\tau = +1$ ($\tau = -1$) (not shown).

We now study the effect of gated region on the reflected electron beam with some parameters different from those in figure 2. The GHL shifts as a function of normalized barrier width $k'_x d$ in the both regimes are shown in figure 3. In the Klein tunneling effect (figures 3(a) and (b)), the reflected $K$ valley electrons exhibit positive or negative values of the lateral shifts, depending on the $d$ values, whereas the GHL shifts of electrons belonging to the $K'$ valley are only negative. In the classical motion regime (figures 3(c) and (d)), however, the reflected $K'$ valley electrons can take positive or negative shift values, whereas the values are solely positive for the reflected beam belonging to the $K$-valley. The peaks in $\sigma_{res}^{\tau,s}$ correspond to the periodical occurrence of transmission resonances, as can be seen in the transmitted beam (see figure 2). Nevertheless, the lateral shift values at the resonance positions for the reflected electron beams are physically meaningless which is due to the fact that the reflection probability, $R = 1 - T$, at these positions is zero. In the vicinity of the resonances, the lateral shift of the reflected beam (similar to that of the transmitted beam) can increase rapidly when the incident angle approaches the critical angles.
As already mentioned, the $\tau \cdot s_z$ symmetry seen in $\sigma_{\text{tr s}}$, does not exist in $\sigma_{\text{tr r}}$. Therefore, the values of lateral shifts for reflected K-valley electrons with spin $s_z$ are different from those for K$'$-valley electrons with spin $\bar{s}_z$. As a result, the reflected electron beams from such electrostatic barriers are fully spin- and valley-polarized. However, as can be seen from figure 3, the lateral shift difference for the reflected electrons with the same value of $\tau \cdot s_z$ (in both regimes) is not enough to be detected experimentally, while it is detectable for electrons with different values of $s_z$, when the incident angle is sufficiently close to $\phi_c$ (not shown).

From equation (6) it is clear that the critical angle $\phi_c$ for incident spin-polarized electrons with energy $E$ is valley-dependent. Figure 4 shows that how this angle for an incident electron with $s_z = +1$ and $\tau = \pm 1$ changes with energy. We can see that the values of $\phi_c$ within a specific energy window are quite different for the two valleys. This suggests that the incident angle $\phi$ can be tuned so that only electrons from a specific valley traverse through the electrostatic barrier, while the electrons from the other valley are fully reflected and blocked. For instance, for electrons with $s_z = +1$ and incident energy $E = 1.75$ eV, the critical angles in two valleys are $\phi_c(\tau = 1) = 50^\circ$ and $\phi_c(\tau = -1) = 20^\circ$ (see figure 4). Therefore, if the incident angle $\phi$ ranges between $20^\circ$ and $50^\circ$, the K$'$ valley electrons are backscattered, while the electrons belonging to the K-valley are transmitted, due to the different trajectories imposed by the gate voltage for each valley, indicating a valley filter with wide tunability.

The energy dependence of GHL shift for the transmitted K and K$'$ valley electrons with $s_z = 1$ through the gated region with $d = 4$ nm is shown in figure 5. The lateral shifts of electrons at various angles of incidence (figures 5(a) and (b)) demonstrate successive peaks with different absolute values, corresponding to the transmission resonances, in both Klein tunneling and classical motion regimes with positive and negative lateral shifts, respectively. The almost zero lateral shift region between Klein tunneling and classical motion is the transmission gap [33] and is given by

$$V_G + \frac{1}{2} \tau s_z \lambda - \frac{1}{2} \sqrt{\left(4a^2 \gamma^2 k_f^2 + (\Delta - \tau s_z \lambda)^2 \right)} < E < V_G + \frac{1}{2} \tau s_z \lambda + \frac{1}{2} \sqrt{\left(4a^2 \gamma^2 k_f^2 + (\Delta - \tau s_z \lambda)^2 \right)} ,$$

which includes the energy gap as well.

Clearly the transmission gap can be wider and the absolute values of the lateral shifts, as well as their difference belonging to different valleys, can be enhanced by increasing the angle of incidence. Moreover, by comparing the energies of maximum absolute values of GHL shifts for K and K$'$ electrons, we can see that the valley separation in the case of Klein tunneling is stronger than that in the classical motion [10]. Figures 5(c) and (d) illustrate the effect of various gate voltages on GHL shift of the transmitted K and K$'$ electrons, when the incident angle is $20^\circ$. Here, one can see that the transmission gap also

5 The transmission gap is an interval of energy where the critical angle is less than the incident angle, so that the electron wave function in the gated region becomes evanescent. See [33].
increases with increasing the external gate. In addition, increasing the gate voltage, the whole spectrum of the lateral shifts moves towards higher energies and the maximum absolute values of the shifts as well as their differences, increase.

Note that due to the time reversal symmetry, the lateral shifts of incident electrons with spin $s_z = -1$, remain unchanged, if we interchange the valleys in the transmitted beam, while the lateral shifts will be somewhat different by interchanging the valleys in the reflected electron beams (not shown) due to the absence of $\tau \cdot s_z$ symmetry, as discussed previously.

In order to explore the influence of a continues range of gate voltages on the GHL shift, in figure 6 we show the calculated results for transmitted K and K' electrons with spin $s_z = 1$ at three different incident angles. The incident energy $E$ and the width $d$ of the gated region are fixed at 2.5 eV and 4 nm, respectively.

Comparing the gate voltages at which the absolute values of the lateral shifts in the two valleys are maximum, we can see that at some gate values the shift of K' valley electrons in the Klein tunneling is almost zero, while the shift of K valley electrons is maximum. As already mentioned, these maximum values correspond to the transmission resonances and demonstrate the valley splitting of charge carriers in WS$_2$ monolayers, which can be generated and controlled by gate voltage [8, 10].

5. Conclusion

In conclusion, the spin-valley transport and the GHL effect of the transmitted and reflected electrons in a WS$_2$ monolayer with a tunable electrostatic barrier have been theoretically studied in both Klein tunneling and classical motion regimes. Interestingly, it was found that the GHL shift of the reflected electrons does not remain invariant under simultaneous interchange of spins and valleys. Therefore, the spin-valley symmetry in the lateral shifts of the reflected electrons from the barrier is different compared to that in the transmitted electrons. The lateral displacement of electron beams can be positive or negative dependent on the width of the gated region and/or incident energy. Our findings show that a valley filter and valley beam splitter can be achieved by tuning the incident angle of electrons and external gate voltage in WS$_2$ monolayers. These features indicate the possibility of manipulating valley index in the TMD monolayers which can be utilized for quantum information applications [10].

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