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Effects of intervalley scattering on the transport properties in one—dimensional valleytronic devices

Jiaojiao Zhou¹, Shuguang Cheng², Wen-Long You¹ & Hua Jiang¹

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Based on a one-dimensional valley junction model, the effects of intervalley scattering on the valley transport properties are studied. We analytically investigate the valley transport phenomena in three typical junctions with both intervalley and intravalley scattering included. For the tunneling between two gapless valley materials, different from conventional Klein tunneling theory, the transmission probability of the carrier is less than 100% while the pure valley polarization feature still holds. If the junction is composed of at least one gapped valley material, the valley polarization of the carrier is generally imperfect during the tunneling process. Interestingly, in such circumstance, we discover a resonance of valley polarization that can be tuned by the junction potential. The extension of our results to realistic valley materials are also discussed.

Valley is a new degree of freedom of the charge carriers. It exists in a crystalline material with energetically degenerate but inequivalent band structures. In recent years, the community have generated extensive interest in manipulating and controlling of the valleys^{1–3}, and thus stimulate a blooming field of valleytronics. A number of materials, including graphene⁴, layered transition metal dichalcogenides⁵ and Weyl semimetal system⁶ etc, are well known hosts of the valleys. Based on them, there are plenty of researches on valleytronics on both theoretical^{1,2,7–24} and experimental sides^{24–33} in the past few years. To be specific, following the theoretical prediction^{2,7,24}, several groups have successfully created valley polarization and detected its signal through the optical pumping by circularly polarized photons^{24–26} and the valley Hall effect^{28–31} in various valley materials, which made a great progress on the valleytronics.

Subsequently, manipulating the transport of valley polarized carriers becomes an important issue in the valleytronics research. Different from the charge and spin degrees of freedom, there is no symmetry to guarantee the conservation of the valleys. In a realistic material, any potential difference, such as disorder, interface mismatch, surface effect and boundary roughness etc, can induce scattering between different valleys, which may lead to the mixture of the valleys²². Transport experiments demonstrate that there is a characteristic length, similar to localization length and phase relaxation length, namely intervalley scattering length, determines the valley-related phenomena. The valley-dependent effects decay exponentially with such length scale^{28–33}. Thus, reducing intervalley scattering is crucial for highly efficient valleytronic devices. However, in most of previous theoretical studies, the intervalley scattering is neglected by concentrating the studies on a single valley or assuming that the potential is smooth enough^{1,2,7,10–13,20,21,23,24}. In this regard, an immediate question is to what extent could the valley transport properties be affected by intervalley scattering in valleytronic devices.

In this paper, we address such an issue on the basis of investigating the valley transport properties in one-dimensional valley material junction devices. By solving the model analytically, the influences of the both intervalley and intravalley scattering on the junctions between two gapless, one gapless and one gapped, and two gapped valley materials are obtained. Due to the intervalley scattering, the Klein tunneling theory, which predicts that the carriers experience a perfect tunneling with 100% transmission probability between two gapless valley materials, is invalid^{34,35}. However, the pure valley polarization feature of the transmitted carriers still holds. If the junctions contain gapped valley materials at least in one terminal, the intervalley scattering always lead to a partial change of the valley polarization during the tunneling process. Under this circumstance, the valley polarization ratio can be manipulated by tuning the junction potential due to the existence of the valley polarization resonance phenomena. Finally, we discuss the extension of our findings to two- and three-dimensional valley materials.

¹College of Physics, Optoelectronics and Energy, Soochow University, Suzhou, 215006, China. ²Department of Physics, Northwest University, Xian 710069, China. Correspondence and requests for materials should be addressed to H.J. (email: jianghuaphy@suda.edu.cn)

Figure 1. Illustration of studied model. (a) Schematic diagram of one-dimensional valley junction device, V_L , V_R are the site potential on the left and right side; (b) illustrates a proposal of orbit and lattice geometries for the realization of our ideal valley model; (c,d) show valley configurations of the model under $\Delta = 0$ (c) and $\Delta \neq 0$ (d). (e) Schematic plot of the a valley tunneling process: an incident valley polarized mode will have two transmitted valley modes with the tunneling coefficients t_1 and t_2 and two reflected valley modes with the reflection coefficients r_1 and r_2 .

Results

Model. To study the valley transport, we begin with constructing a minimal lattice model. As sketched in Fig. 1(a,b), we consider a junction device with one-dimensional valley materials on both sides. In the tight-binding representation, the effective Hamiltonian can be written as:

$$H = H_L + H_R + H_{LR}, \quad (1)$$

in which

$$\begin{aligned} H_L &= \sum_{n \leq 0} [U_L(S_{n-1}^+ P_n - P_{n-1}^+ S_n) + h.c. + (V_L + \Delta_L) S_n^+ S_n + (V_L - \Delta_L) P_n^+ P_n], \\ H_R &= \sum_{n \geq 1} [U_R(S_n^+ P_{n+1} - P_n^+ S_{n+1}) + h.c. + (V_R + \Delta_R) S_n^+ S_n + (V_R - \Delta_R) P_n^+ P_n], \\ H_{LR} &= J_0(S_1^+ P_0 - P_1^+ S_0) + h.c. \end{aligned}$$

Here H_L , H_R and H_{LR} describe the left side, the right side and the tunneling coupling in between, respectively. There are two orbits S , P_x for each site n and S_n , P_n denote the corresponding annihilation operators. V_L (V_R) characterizes the on-site potential and Δ_L (Δ_R) specifies the site potential difference of these two orbits on left (right) side. We assume that the electron hopping can only happen between the S orbit and the nearest-neighbor site P_x orbits [see Fig. 1]. J_L , J_R and J_0 are the hopping energies on the left side, the right side and the junction interface, respectively. We note that our minimal model can be realized in the special ultracold atom systems, where every parameter in the Hamiltonian can be tuned physically (please see ref. 36 for details). In the following, we set $J_L = J_R = 1$, $V_L = 0$ and $V_R = V$ for convenience.

We perform a Fourier transformation to Eq. (1) and obtain its form in the momentum space:

$$H(k) = \begin{pmatrix} V + \Delta & 2iJ \sin k \\ -2iJ \sin k & V - \Delta \end{pmatrix}. \quad (2)$$

For simplicity, we have set the lattice constant $a = 1$. $H(k)$ has two eigenvalues $\epsilon_{\pm} = V \pm \sqrt{\Delta^2 + 4J^2} \sin^2 k$, where ϵ_+ (ϵ_-) corresponds to the conduction (valence) band. Figure 1(c) plots the energy dispersion of $H(k)$ for $\Delta = 0$ and $\Delta \neq 0$. The energy band are degenerate at $k = 0$ (K) and $k = \pi$ (K'), which means that there exist two inequivalent valley K and K' . Moreover, two types of valleys can be realized by tunneling Δ . One type is gapless as illustrated in Fig. 1(c) and the other has gapped spectrum in Fig. 1(d). In a word, the minimal model provides a platform to study the valley transport properties between the valley materials, in both gapless and gapped situations.

In the following, we focus on the valley transport properties for the junction devices. The incident carriers are purely K -valley polarized. The valley-resolved transmission probabilities T_{KK} , $T_{KK'}$, reflection probabilities

Figure 2. Valley-resolved transmission probabilities T_{KK} (a), $T_{KK'}$ (c) and reflection probabilities $R_{KK'}$ (b), R_{KK} (d) versus Fermi energy E for different interfacial hopping energy J_0 . The interfacial potential of the junction is fixed to $V = 0.5$. The hopping energies on both sides of the junction are $J_L = J_R = 1$.

R_{KK} , $R_{KK'}$, the total transmission probability T and the valley polarization ratio P are obtained analytically. See **Methods** for details of these calculations.

In recent years, lots of gapless or gapped valley materials have been discovered. In general, three types of valley junction can be built through these materials: gapless junction between two gapless valley materials ($\Delta_L = \Delta_R = 0$); hybridized junction with gapless and gapped valley materials ($\Delta_L = 0, \Delta_R \neq 0$ or $\Delta_L \neq 0, \Delta_R = 0$); gapped junction between two gapped valley materials ($\Delta_L \neq 0, \Delta_R \neq 0$). Without loss of generality, we consider these three cases separately.

$$\Delta_L = \Delta_R = 0$$

In this subsection, we study the transport properties of a junction between two gapless valley materials. The considered situation is analogue to the valley transport properties in graphene, silicene, and germanene PN junction etc.^{37,38}. Conventionally, the Klein tunneling theory is used to describe the transport phenomena in the gapless material systems^{34,35,39}. In such theory, only single valley is considered. Thus, due to the absence of intervalley scattering, the valley polarization will never be changed during the scattering processes ($P = 1$). Moreover, the gapless feature forbids the intravalley backscattering ($r = 0$, see the second part of section **Methods**). The carrier can tunnel through the barrier freely ($T = 1$). However, in real materials, the *fermion doubling theorem* guarantees that the gapless valleys exist in pairs⁴⁰. Thus, the intervalley scattering is unavoidable due to the interfacial complexity.

To show an intuitive picture for the influence of intervalley scattering, we firstly study the junction in an extreme condition that large mismatch exists at the interface, that is, the hopping energy J_0 is much different from J_L, J_R . Figure 2 plots the valley resolved probability T_{KK} (a), $R_{KK'}$ (b), $T_{KK'}$ (c) and R_{KK} (d) versus the Fermi energy E for different hopping energy J_0 . At first glance, $T_{KK'}$ and R_{KK} are equal to zero, independent with J_0 and E . $T_{KK'} = 0$ means that the K valley polarized carriers on left side cannot tunnel into the K' valley on the right side. Thus, the valley polarization ($P = 1$) will not be changed during the tunneling processes. $R_{KK} = 0$ implies that the K valley carriers cannot be reflected back to its own valley. These two features agree well with the Klein theory. But, in such gapless system, the total transmission probability ($T = T_{KK} = 1$) predicted in Klein theory is violated. As shown in Fig. 2(a), T_{KK} is not equal to 1. By decreasing J_0 , $T = T_{KK}$ drop quickly. This phenomenon stems from the fact that the intervalley scattering is allowed for the existence of pairs of valleys. As seen from Fig. 2(b), the K valley carrier can be reflected to the K' valley. A decrease of J_0 leads to a rapid increase of $R_{KK'}$.

J_0 is not the only mechanism that can cause the intervalley scattering. Even though $J_0 = J_L = J_R$, intervalley scattering still emerges by tuning the junction potential V . In the following, we will focus on this case, because it is much closer to the experimental situation. We find that the influence of V for a single junction is weak. However, in realistic experimental situations, the carriers may experience a series of junctions during the tunneling process, thus the influence of V will be enhanced.

Figures 3 and 4 show the relationship about transmission probabilities T_{KK} (a), $T_{KK'}$ (c) and reflection probabilities $R_{KK'}$ (b), R_{KK} (d) with the Fermi energy E and the potential V . In Figs 3(c,d) and 4(c,d), $T_{KK'}$ and R_{KK} still equal to zero, as same as those in Fig. 2(c,d). This phenomenon indicates that the valley polarization cannot be changed ($T_{KK'} = 0$ and $P = 1$) during the tunneling processes. By changing the potential V or the Fermi energy E , the probability that the K -polarized carriers tunnel into the valley K ($T_{KK} \neq 1$) or been reflected into the valley K' ($R_{KK'} \neq 0$) can be adjusted. As plotted in Fig. 3, T_{KK} has an obvious decrease and $R_{KK'}$ shows an obvious increase with respect to large V . In contrast, in Fig. 4, T_{KK} and $R_{KK'}$ change slowly by varying the Fermi energy E . These two behaviors can be understood by the analytic expression of $R_{KK'}$ under the situation $\Delta_L = \Delta_R = 0$. From Eqs (9) and (10), one obtains

Figure 3. Transmission probabilities T_{KK} (a), $T_{KK'}$ (c) and reflection probabilities $R_{KK'}$ (b), R_{KK} (d) vs Fermi energy E for different potential $V = 0.0, 0.2, 0.4, 0.6, 0.8$. All hopping energies are set to be equal, $J_0 = J_L = J_R = 1$.

Figure 4. Transmission probabilities T_{KK} (a), $T_{KK'}$ (c) and reflection probabilities $R_{KK'}$ (b), R_{KK} (d) versus potential V for different Fermi energy $E = 0.0001, 0.1, 0.2, 0.4$. The hopping energies are the same as Fig. 3.

$$R_{KK'} = \left[\frac{\sin((k_L - k_R)/2)}{\cos((k_L + k_R)/2)} \right]^2. \quad (3)$$

When Fermi level E is near the Dirac point, both k_L and k_R are very small. The junction keeps a linear dispersion on both sides. As a consequence, $k_L - k_R$ is proportional to the potential V and $\cos(k_L + k_R)$ is insensitive to the variation of Fermi energy E . Therefore, T_{KK} and $R_{KK'}$ are sensitive to the potential V due to the rapid variation of $k_L - k_R$. When V is fixed and the energy structure is in linear dispersion regime, T_{KK} and $R_{KK'}$ change slowly with E due to small variation of $\cos(k_L + k_R)$. When E is shifted away from the linear dispersion regime, the total transmission probability $T = T_{KK}$ deviates significantly from unit.

$$\Delta_L \neq 0, \Delta_R = 0 \text{ or } \Delta_L = 0, \Delta_R \neq 0$$

In this subsection, we study transport properties of a junction in which only one side has gapped valleys. In this circumstance, valley-polarized carriers are injected from gapless valley materials to gapped valley materials or vice versa. This hybrid junction can be realized in experiments. For example, we can design a junction composing of a monolayer MoS_2 hybridized with graphene sheet or a junction for bilayer graphene with unbiased left side and biased right side⁴¹.

In Figs 5 and 6, T_{KK} , $T_{KK'}$, R_{KK} , $R_{KK'}$ as a function of potential V for gapped valleys on left-side (Fig. 5) or right-side (Fig. 6) of junction are plotted, respectively. The corresponding probabilities of the gapless junction studied in the above subsection ($\Delta_L = \Delta_R = 0$) are also plotted in these two figures (black square curves) for comparison. Remarkably, when either $\Delta_L \neq 0$ or $\Delta_R \neq 0$, both $T_{KK'}$ and R_{KK} are always nonvanishing. Owing to the existence of the additional intravalley backscattering, the transmission probabilities T is weakened. More importantly, with the occurrence of the intervalley transmission, the valley polarization ratio P is less than the unit. In the following, we investigate how T and P are affected in detail.

Figure 5. The valley resolved transmission probabilities T_{KK} (a), $T_{KK'}$ (d), total transmission probabilities T (c), reflection probabilities $R_{KK'}$ (b), R_{KK} (e) and valley polarization ratio P (f) versus interfacial potential V . The valley gap on the left side equal to 0.0, 0.1, 0.2, 0.3, respectively. The other parameters are set as: the valley gap on the right side $\Delta_R = 0$, the Fermi energy $E = 0.5$ and the hopping energy $J_0 = J_L = J_R = 1$. Inset of (f) is the schematic diagram for the carrier tunneling process.

Figure 6. The valley resolved transmission probabilities T_{KK} (a), $T_{KK'}$ (d), the transmission probabilities T (c), reflection probabilities $R_{KK'}$ (b), R_{KK} (e) and the valley polarization ratio P (f) versus interfacial potential V . The valley gap is on the right side, $\Delta_L = 0$, $\Delta_R \neq 0$. The Fermi energy E and the hopping energies J_0, J_L, J_R are the same as those in Fig. 5. Inset of (f): schematic of the tunneling process for valley polarized carriers.

In Fig. 5(c), the transmission probabilities T under different valley gap Δ_L and potential V are plotted. T decrease rapidly by increasing the gap Δ_L and the potential V . The variation of T versus Δ_L is mainly contributed by the dominant reduction of T_{KK} for larger Δ_L . It can be understood by the transport theory with single valley (see section **Methods** for detail). Meanwhile, the variation of T versus V follows its tendency at $\Delta_L = 0$ (black line). The phenomena originates from the same mechanism that a rise of V will sharply enhance the intervalley scattering $R_{KK'}$ (see Fig. 5(b)). Furthermore, the relationship of valley-polarization ratio P versus potential V for different Δ_L are shown in Fig. 5(f). First, in the present model, no perfect valley polarization can be realized as long as $\Delta_L > 0$. Second, P is proportional to V while in inverse proportion to Δ_L . Such relationship is determined by the variation of $T_{KK'}$ versus V and T . For fixed potential V , the band structure on the both sides of the junction becomes more asymmetrical by increasing of Δ_L , leading to an enhancement of $T_{KK'}$. In contrast, by increasing V , $T_{KK'}$ decreases since the band structure on the both sides of the junction becomes more symmetrical. From above relationship, one can conclude that the polarization ratio P can be manipulated by controlling V . To be specific, for fixed Δ_L , the valley-polarization P can be greatly improved with little expense of T by increasing V .

In Fig. 6(c,f), we investigate the case that nonzero valley gaps only emerge on the right side of the junction. Comparing with the curves that Fermi energy shifts from the valence band to the conduction band, the behaviors of T and P are nearly the same. In other words, both T and P are insensitive to the type of carriers (p/n). Further, when Fermi energy E approaches the band gap, both transmission probabilities T and valley polarization ratio P

Figure 7. The total transmission probability T (a–d), and the valley polarization ratio P (e–h) as functions of V and the valley gap on the right side Δ_R . (a,e), (b,f), (c,g) and (d,h) correspond to $\Delta_L = 0.0, 0.1, 0.2, 0.3$. The other parameters are the same as those in Fig. 5. Inset of (h) illustrates the valley tunneling process.

Figure 8. The valley-resolved probability $T_{KK'}$ versus potential V in the case of $\Delta_L = 0.3$ and $\Delta_R = 0.2$. The other parameters are the same as those in Fig. 5.

decrease rapidly. From the relationship of P versus Δ_L and V (see Fig. 6(f)), it is also worth emphasizing that, due to the intervalley scattering, the valley polarization ratio P is generally less than unit. Meanwhile, one can also manipulate P by adjusting the potential V .

$$\Delta_L \neq 0 \text{ and } \Delta_R \neq 0$$

After the discovery of series of gapped valley materials recently^{3,5}, great interest has been sparked in the study of valley transport in these materials. In this subsection, we study the transport properties of a junction between two gapped valley materials.

Figure 7 plots the transmission probabilities T and the valley polarization ratio P versus potential V for different band gaps. Main features of relationship between T , P and V , Δ are obtained. In general, due to the intervalley scattering, P is less than 1, indicating that partial carriers will change their valley; T is not identical to 1, which means that the backscattering takes place at the interface; T and P decrease rapidly at the gap edges.

Interestingly, in the presence of gapped valley materials, resonance phenomena happen to P (see Figs 5 and 7). In other words, at some special values of V (e.g., $V = 0.167$ or $V = 0.947$ in Fig. 7(h)), the valley polarization will not be changed during the tunneling process ($P = 1$). We have carefully investigated such resonance phenomenon since it may have potential application in the manipulation of valley transport.

Physically, the P resonance is caused by the vanishment of intervalley transmission probability $T_{KK'}$. Figure 8 illustrates $T_{KK'}$ as a function of V . One can see two zero points for $T_{KK'}$. After some algebras, we find that the resonance points locate at

$$V = E + \sqrt{E^2 + \Delta_R^2 - \Delta_L^2}, \quad (4)$$

or

$$V = \frac{\Delta_L - \Delta_R}{\Delta_L} E. \quad (5)$$

Noting the first type valley resonance phenomenon [Eq. (4)] can also exist in the hybridized junction that only $\Delta_L = 0$ or $\Delta_R = 0$. In contrast, the second type valley resonance phenomenon [Eq. (5)] can only exist in the junction with gapped valleys on both sides ($\Delta_L \neq 0$ and $\Delta_R \neq 0$). To be specific, when Δ_L approaches Δ_R , a pure valley polarization can easily be obtained by slightly tuning the potential V . Equation (5) is the master equation that determines such valley manipulation.

Discussion and Conclusion

Commonly, the valley materials that have been successfully fabricated in experiments are two- or three-dimensional with complicated electric structure^{42–45}. In the main text, we concentrate our studies on a simple one-dimensional valley junction model. However, the underlying physical mechanism of the valley transport properties even in the complicated materials has been clearly demonstrated in such a simple model. Taking a junction composed of two-dimensional gapless valley materials (e.g. monolayer graphene) for example, its momentum can be decoupled into the perpendicular component $k_\perp$ and the parallel component $k_\parallel$ along the junction interface. The eigenvalues and eigenstates are similar to those in Eq. (2) except that Δ is replaced by the momentum $k_\parallel$. Due to the continuity relationship of the wavefunction, Eq. (9) still holds and $k_\parallel$ remains unchanged across the junction. Therefore, for normally incident carriers, their valley transport should show similar behaviors as elaborated in subsection $\Delta_L = \Delta_R = 0$. For carriers with an incident angle, their valley transport properties should share similar features to those observed in subsection $\Delta_L \neq 0$ and $\Delta_R \neq 0$ with $k_\parallel = \Delta_L = \Delta_R$. Parallel analysis can be applied to the two-dimensional gapped valley materials and three-dimensional valley materials, and their valley transport properties will resemble the last three subsections in Results, depending on the initial condition. Conclusively, our analytic results can also characterize the main features of valley transport phenomena in both two- and three-dimensional valley materials.

In summary, the valley transport properties of a junction between one-dimensional materials with gapless (or gapped) valleys are studied. Our analytic results have clearly shown that the strong intervalley scattering, which is always omitted in the previous theory, can greatly influence the valley transport properties of valleytronic devices. Concretely, for a junction with two gapless valley materials, the intervalley scattering can cause the reflection of the tunneling carriers and damage the perfect tunneling. Nevertheless, the valley polarization of the carriers remains unchanged in such a case. In contrast, for a junction containing gapped valley materials, the valley polarization of the carriers can be changed during the tunneling process. Besides, we discover a valley polarization resonance phenomena and extract the corresponding condition, which may be utilized to manipulate the valley degree in the future.

Methods

Valley transport with intervalley scattering included. As shown in Fig. 1(e), for the incident mode Φ_{in} , there are two reflection modes Φ_{r1}, Φ_{r2} on the left side and two transmission modes Φ_{t1}, Φ_{t2} on the right side. $\Phi_{in}, \Phi_{r1}, \Phi_{r2}, \Phi_{t1}, \Phi_{t2}$ on site n are given by:

$$\begin{aligned} \Phi_{in}^n &= \sqrt{\frac{\hbar}{4J_L A_L \cos k_L}} e^{ik_L n} \begin{pmatrix} 1 \\ iA_L \end{pmatrix}, \\ \Phi_{r1}^n &= \sqrt{\frac{\hbar}{4J_L A_L \cos k_L}} e^{-ik_L n} \begin{pmatrix} 1 \\ -iA_L \end{pmatrix}, \quad \Phi_{r2}^n = \sqrt{\frac{\hbar}{4J_L A_L \cos k_L}} e^{-i(k_L + \pi)n} \begin{pmatrix} 1 \\ iA_L \end{pmatrix}, \\ \Phi_{t1}^n &= \sqrt{\frac{\hbar}{4J_R A_R \cos k_R}} e^{ik_R n} \begin{pmatrix} 1 \\ iA_R \end{pmatrix}, \quad \Phi_{t2}^n = \sqrt{\frac{\hbar}{4J_R A_R \cos k_R}} e^{i(k_R + \pi)n} \begin{pmatrix} 1 \\ -iA_R \end{pmatrix}, \end{aligned} \quad (6)$$

where $k_L(k_R)$ represents the wavevector of the mode $\Phi_{in}(\Phi_{t1})$ at Fermi energy E . The components $A_L = -(E - \Delta_L)/(\sqrt{E^2 - \Delta_L^2})$ and $A_R = \eta(E - V - \Delta_R)/(\sqrt{(E - V)^2 - \Delta_R^2})$. Here $\eta = -1(1)$ corresponds to the case that E is located in the conduction band or the band gap (the valence band). A_R is purely imaginary when E is located inside the band gap. The two-component spinors in Eq. (6) originate from the eigenvector of $H(k)$. It is worth noting that, in order to satisfy the unitary properties of scattering matrix, all modes in Eq. (6) have been normalized by the current operator $j = \partial H(k)/\partial k$.

The wave function Ψ_n at site n can be written as a combination of the incident modes and reflected/transmitted modes in the following equations:

$$\Psi_n = \begin{cases} \Phi_{in}^n + r_1 \Phi_{r1}^n + r_2 \Phi_{r2}^n, & n \leq 0; \\ t_1 \Phi_{t1}^n + t_2 \Phi_{t2}^n, & n \geq 1. \end{cases} \quad (7)$$

From the stationary Schrödinger equation, $H\Psi = E\Psi$, the continuity relationship across the interface can be expressed as:

$$\begin{aligned} H_{0-1}\Psi_{-1} + H_{00}\Psi_0 + H_{01}\Psi_1 &= E\Psi_0, \\ H_{10}\Psi_0 + H_{11}\Psi_1 + H_{12}\Psi_2 &= E\Psi_1. \end{aligned} \quad (8)$$

Combining Eqs (6) and (8), we have

$$\begin{aligned}
 t_1 &= \frac{A_L(1 + e^{2ik_L})}{2x} \left[\frac{1}{JA_R e^{i(k_L+k_R)} + A_L J^{-1}} + \frac{1}{JA_L e^{i(k_L+k_R)} + A_R J^{-1}} \right], \\
 t_2 &= \frac{A_L(1 + e^{2ik_L})}{2x} \left[\frac{1}{JA_R e^{i(k_L+k_R)} + A_L J^{-1}} - \frac{1}{JA_L e^{i(k_L+k_R)} + A_R J^{-1}} \right], \\
 r_1 &= \frac{1 + e^{2ik_L}}{2J} \left[\frac{A_L}{J^{-1}A_L + JA_R e^{i(k_L+k_R)}} - \frac{A_R}{J^{-1}A_R + JA_L e^{i(k_L+k_R)}} \right], \\
 r_2 &= \frac{1 + e^{2ik_L}}{2J} \left[\frac{A_L}{J^{-1}A_L + JA_R e^{i(k_L+k_R)}} + \frac{A_R}{J^{-1}A_R + JA_L e^{i(k_L+k_R)}} \right] - 1,
 \end{aligned} \tag{9}$$

where $x = \sqrt{A_L \cos k_L / (A_R \cos k_R)}$ and $J = \sqrt{J_0^2 / (J_L J_R)}$. Consequently, we can get the corresponding transmission and reflection probabilities:

$$\begin{aligned}
 T_{KK} &= |t_1|^2, \quad T_{KK'} = |t_2|^2, \\
 R_{KK} &= |r_1|^2, \quad R_{KK'} = |r_2|^2.
 \end{aligned} \tag{10}$$

$T_{KK}(T_{KK'})$ denotes the transmission probability of carriers from K valley on the left side to the $K(K')$ valley on the right side, and $R_{KK}(R_{KK'})$ represents the reflection probabilities of carriers from K valley to $K(K')$ valley. It could be proved that $T_{KK} + T_{KK'} + R_{KK} + R_{KK'} = 1$. Such constraint is guaranteed by the unitary properties of the scattering matrices and shows strong confirmation of our analytical derivations.

Based on the valley-resolved transmission probability, we can define the total transmission probability

$$T = T_{KK} + T_{KK'}, \tag{11}$$

and the valley polarization ratio

$$P = \frac{T_{KK} - T_{KK'}}{T_{KK} + T_{KK'}}. \tag{12}$$

T and P are two important quantities characterize the valley transport properties of the device.

Single valley transport theory. For single valley model, the low-energy effective Hamiltonian can be written as:

$$H = \begin{bmatrix} V + \Delta & \mathbf{k} \\ \mathbf{k} & V - \Delta \end{bmatrix} \tag{13}$$

The above Hamiltonian have eigenvalues $E = V \pm \sqrt{\Delta^2 + \mathbf{k}^2}$. For simplicity, we focus on conduction band $E = V + \sqrt{\Delta^2 + \mathbf{k}^2}$ and its eigenfunction is $\begin{pmatrix} 1 \\ \frac{E - V - \Delta}{\sqrt{(E - V)^2 - \Delta^2}} \end{pmatrix}^T$.

We consider a junction with gapless left side ($\Delta_L = 0$) and gapped right side ($\Delta_R \neq 0$). The continuity of wavefunction across the boundary can be written as:

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} + r \begin{pmatrix} 1 \\ -1 \end{pmatrix} = t \begin{pmatrix} 1 \\ \frac{E - V - \Delta_R}{\sqrt{(E - V)^2 - \Delta_R^2}} \end{pmatrix} \tag{14}$$

Finally, we obtain the reflection amplitude

$$r = \frac{\sqrt{(E - V)^2 - \Delta_R^2} - E + V + \Delta_R}{E - V - \Delta_R + \sqrt{(E - V)^2 - \Delta_R^2}}. \tag{15}$$

When $\Delta_R = 0$, $r = 0$ for arbitrary V . It corresponds to the total transmission, which is in agreement with Klein theory for massless fermion system. In contrast, when $\Delta_R \rightarrow E - V$, the reflection amplitude $r \rightarrow 1$. It corresponds to the perfect reflection.

References

1. Rycerz, A., Tworzydło, J. & Beenakker, C. W. J. Valley filter and valley valve in graphene. *Nature Phys.* **3**, 172 (2006).
2. Niu, Q., Xiao, D. & Yao, W. Valley-Contrasting Physics in Graphene: Magnetic Moment and Topological Transport. *Phys. Rev. Lett.* **99**, 236809 (2007); Valley-dependent optoelectronics from inversion symmetry breaking. *Phys. Rev. B* **77**, 235406 (2008).
3. Xu, X., Yao, W., Xiao, D. & Heinz, T. F. Spin and pseudospins in layered transition metal dichalcogenide. *Nature Phys.* **10**, 343 (2014).
4. Neto, A. H. C., Guinea, F., Peres, N. M. R., Novoselov, K. S. & Geim, A. K. The electronic properties of graphene. *Rev. Mod. Phys.* **81**, 109 (2009).
5. Mak, K. F., Lee, C., Hone, J., Shan, J. & Heinz, T. F. Atomically thin MoS₂: a new direct-gap semiconductor. *Phys. Rev. Lett.* **105**, 136805 (2010).
6. Hosur, P. & Qi, X. L. Recent developments in transport phenomena in Weyl semimetals. *C. R. Physique* **14**, 857 (2013).

7. Xiao, D., Liu, G. B., Feng, W. X., Xu, X. D. & Yao, W. Coupled Spin and Valley Physics in Monolayers of MoS₂ and Other Group-VI Dichalcogenides. *Phys. Rev. Lett.* **108**, 196802 (2012).
8. Lopes, P. L. e S., Neto, A. H. C. & Caldeira, A. O. Chiral filtering in graphene with coupled valleys. *Phys. Rev. B* **84**, 245432 (2011).
9. Garcia-Pomar, J. L., Cortijo, A. & Vesperinas, M. N. Fully Valley-Polarized Electron Beams in Graphene. *Phys. Rev. Lett.* **100**, 236801 (2008).
10. Gunlycke, D. & White, C. T. Graphene Valley Filter Using a Line Defect. *Phys. Rev. Lett.* **106**, 136806 (2011).
11. Zhai, F., Zhao, X. F., Chang, K. & Xu, H. Q. Magnetic barrier on strained graphene: A possible valley filter. *Phys. Rev. B* **82**, 115442 (2010).
12. Low, T. & Guinea, F. Strain-Induced Pseudomagnetic Field for Novel Graphene Electronics. *Nano Lett.* **10**, 3551 (2010).
13. Zhai, F., Ma, Y. L. & Chang, K. Valley beam splitter based on strained graphene. *New J. Phys.* **13**, 083029 (2011).
14. Zhang, F., Jung, J., Fiete, G. A., Niu, Q. & MacDonald, A. H. Spontaneous Quantum Hall States in Chirally Stacked Few-Layer Graphene Systems. *Phys. Rev. Lett.* **106**, 156801 (2011).
15. Zhu, Z., Collaudin, A., Fauque, B., Kang, W. & Behnia, K. Field-induced polarization of Dirac valleys in bismuth. *Nature Phys.* **8**, 89 (2012).
16. Zhang, F., MacDonald, A. H. & Mele, E. J. Valley Chern numbers and boundary modes in gapped bilayer graphene. *Proc. Natl. Acad. Sci. USA* **110**, 10546 (2013).
17. Liu, Y., Song, J. T., Li, Y. X., Liu, Y. & Sun, Q. F. Controllable valley polarization using graphene multiple topological line defects. *Phys. Rev. B* **87**, 195445 (2013).
18. Qiao, Z. H., Jung, J., Niu, Q. & MacDonald, A. H. Electronic highways in bilayer graphene. *Nano Lett.* **11**, 3453 (2011).
19. Pan, H., Li, X., Jiang, H., Yao, Y. G. & Yang, S. Y. Valley-polarized quantum anomalous Hall phase and disorder induced valley filtered chiral edge channels. *Phys. Rev. B* **91**, 045404 (2015).
20. Jiang, H., Liu, H. W., Feng, J., Sun, Q. F. & Xie, X. C. Transport discovery of emerging robust helical surface states in Z₂ = 0 systems. *Phys. Rev. Lett.* **112**, 176601 (2014).
21. Jiang, Q. D., Jiang, H., Liu, H. W., Sun, Q. F. & Xie, X. C. Topological Imbert-Fedorov shift in Weyl semimetals. *Phys. Rev. Lett.* **115**, 156602 (2015).
22. Liu, G.-B., Pang, H. L., Yao, Y. G. & Yao, W. Intervalley coupling by quantum dot confinement potentials in monolayer transition metal dichalcogenides. *New J. Phys.* **16**, 105011 (2014).
23. Qi, J. S., Li, X., Niu, Q. & Feng, J. Giant and tunable valley degeneracy splitting in MoTe₂. *Phys. Rev. B* **92**, 121403 (2015); Li, X., Cao, T., Niu, Q., Shi, J. R. & Feng, J. Coupling the valley degree of freedom to antiferromagnetic order. *Proc. Natl. Acad. Sci. USA* **110**, 3738 (2013).
24. Cao, T., Wang, G., Han, W. *et al.* Valley-selective circular dichroism of monolayer molybdenum disulphide. *Nat. Commun.* **3**, 887 (2012).
25. Zeng, H., Dai, J., Yao, W., Xiao, D. & Cui, X. Valley polarization in MoS₂ monolayers by optical pumping. *Nature Nanotech.* **7**, 490 (2012).
26. Mak, K. F., He, K., Shan, J. & Heinz, T. F. Control of valley polarization in monolayer MoS₂ by optical helicity. *Nature Nanotech.* **7**, 494 (2012).
27. Chen, J. H., Autès, G., Alem, N., Gargiulo, F., Gautam, A., Linck, M., Kisielowski, C., Zayzev, O. V., Louie, S. G. & Zettl, A. Controlled growth of a line defect in graphene and implications for gate-tunable valley filtering. *Phys. Rev. B* **89**, 121407(R) (2014).
28. Mak, K. F., McGill, K. L., Park, J. & McEuen, P. L. The valley Hall effect in MoS₂ transistors. *Science* **344**, 1489 (2014).
29. Gorbachev, R. V. *et al.* Detecting topological currents in graphene superlattices. *Science* **346**, 448 (2014).
30. Sui, M., Chen, G., Ma, L., Shan, W., Tian, D., Watanabe, K., Taniguchi, T., Jin, X., Yao, W., Xiao, D. & Zhang, Y. Gate-tunable topological valley transport in bilayer graphene. *Nature Phys.* **11**, 1027 (2015).
31. Shimazaki, Y., Yamamoto, M., Borzenets, I. V., Watanabe, K., Taniguchi, T. & Tarucha, S. Generation and detection of pure valley current by electrically induced Berry curvature in bilayer graphene. *Nature Phys.* **11**, 1032 (2015).
32. Ju, L., Shi, Z., Nair, N., Lv, Y. C. *et al.* Topological valley transport at bilayer graphene domain walls. *Nature* **520**, 650 (2015).
33. Li, J., Wang, K., McFaul, K. J., Zern, Z., Ren, Y. F., Watanabe, K., Taniguchi, T., Qiao, Z. H. & Zhu, J. Experimental observation of edge states at the line junction of two oppositely biased bilayer graphene. arXiv: 1509.03912.
34. Katsnelson, M. I., Novoselov, K. S. & Geim, A. K. Chiral tunnelling and the Klein paradox in graphene. *Nature Phys.* **2**, 620 (2006).
35. Cheianov, V. V. & Fal'ko, V. I. Selective transmission of Dirac electrons and ballistic magnetoresistance of np junctions in graphene. *Phys. Rev. B* **74**, 041403 (2006).
36. Li, X., Zhao, E. & Liu, W. V. Topological states in a ladder-like optical lattice containing ultracold atoms in higher orbital bands. *Nat. Commun.* **4**, 1523 (2013).
37. Ohta, T., Bostwick, A., Seyller, T., Horn, K. & Rotenberg, E. Controlling the electronic structure of bilayer graphene. *Science* **313**, 951 (2006).
38. Yamakage, A., Ezawa, M., Tanaka, Y. & Nagaosa, N. Charge transport in pn and npn junctions of silicene. *Phys. Rev. B* **88**, 085322 (2013).
39. Calogeracos, A. & Dombey, N. History and physics of the Klein paradox. *Contemp. Phys.* **40**, 313 (1999).
40. Nielsen, H. B. & Ninomiya, N. Absence of neutrinos on a lattice: (I). Proof by homotopy theory. *Nucl. Phys. B* **185**, 20 (1981).
41. Zhang, Y., Tang, T. T., Girit, C., Hao, Z., Martin, M. C., Zettl, A., Crommie, M. F., Shen, Y. R. & Wang, F. Direct observation of a widely tunable bandgap in bilayer graphene. *Nature* **459**, 820 (2009).
42. Novoselov, K. S., Geim, A. K., Morozov, S. V., Jiang, D., Zhang, Y., Dubonos, S. V., Grigorieva, I. V. & Firsov, A. A. Electric field effect in atomically thin carbon films. *Science* **306**, 666 (2004).
43. Novoselov, K. S. *et al.* Two-dimensional atomic crystals. *Proc. Natl. Acad. Sci. USA* **102**, 10451 (2005).
44. Isberg, J. *et al.* Generation, transport and detection of valley-polarized electrons in diamond. *Nature Mater.* **12**, 760 (2013).
45. Xu, S. *et al.* Discovery of a Weyl Fermion Semimetal and Topological Fermi Arcs. *Science* **349**, 613 (2015); Lv, B. Q. *et al.* Experimental Discovery of Weyl Semimetal TaAs. *Phys. Rev. X* **5**, 031013 (2015).

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Author Contributions

J.J.Z. and H.J. carried out the theoretical calculations and wrote the manuscript with the assistance of S.-G.C. and W.-L.Y. All authors reviewed the manuscript.

Additional Information

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