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

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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 valleys¹-³, 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 theoretical¹,²,⁷-²⁴ and experimental sides²⁴-³³ in the past few years. To be specific, following the theoretical prediction²,⁷,²⁴, several groups have successfully created valley polarization and detected its signal through the optical pumping by circularly polarized photons²⁴-²⁶ and the valley Hall effect²⁸-³¹ 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 scale²⁸-³³. 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 enough¹,²,⁷,¹⁰-¹³,¹⁷,¹⁸,²⁴. 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 invalid¹⁴,³⁵. 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.

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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:

\[ H = H_L + H_R + H_{LR}, \]

in which

\[ H_L = \sum_{n<0} J_L (S_{n+1}^+ P_n - P_{n+1}^+ S_n) + \text{h.c.} + (V_L + \Delta_L) S_n^+ S_n + (V_L - \Delta_L) P_n^+ P_n, \]
\[ H_R = \sum_{n>1} J_R (S_{n-1}^+ P_{n-1} - P_{n-1}^+ S_{n-1}) + \text{h.c.} + (V_R + \Delta_R) S_{n-1}^+ S_{n-1} + (V_R - \Delta_R) P_{n-1}^+ P_{n-1}, \]
\[ H_{LR} = J_0 (S_1^+ P_0 - P_1^+ S_0) + \text{h.c.}. \]

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 \( S, P \) for each site \( n \) and \( S_n, P_n \) denote the corresponding annihilation operators. \( V_L(V_R) \) characterizes the on-site potential and \( \Delta_L(\Delta_R) \) 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 \( P_i \) 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:

\[ H(k) = \begin{pmatrix} V + \Delta & 2i f \sin k \\ -2i f \sin k & V - \Delta \end{pmatrix}. \]

For simplicity, we have set the lattice constant \( a = 1 \). \( H(k) \) has two eigenvalues \( \epsilon_{\pm} = V \pm \sqrt{\Delta^2 + 4f^2} \sin^2 k \)

where \( \epsilon_{\pm}(\epsilon_c) \) 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 \( \Delta \). 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
and (10), one obtains the intervalley scattering is allowed for the existence of pairs of valleys. As seen from Fig. 2(b), the $K'$ can be reflected to the valley. A decrease of $\Delta$ for details of these calculations.

**Methods**

hybridized junction with gapless and gapped valley materials ($\Delta$) versus Fermi energy $E$ for different interfacial hopping energy $J_0$ in realistic experimental situations, the carriers may experience a series of junctions during the tunneling process, much closer to the experimental situation. We find that the influence of $V$ for a single junction is weak. However, two behaviors can be understood by the analytic expression of RKKY.

Valley-resolved transmission 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.Conventionally, the Klein tunneling theory is used to describe the transport phenomena in the gapless material systems. In such theory, only single valley is considered. Thus, due to the absence of inter-valley 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 pairs. 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 into 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 $J_L = J_R = J_0$, 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
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.

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 consisting of a monolayer MoS$_2$ hybridized with graphene sheet or a junction for bilayer graphene with unbiased left side and biased right side\cite{41}.

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 intervalley transmission, 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.

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

(3)
In Fig. 5(c), the transmission probabilities $T_{KK}$ under different valley gap $\Delta_L$ and potential $V$ are plotted. $T_{KK}$ decrease rapidly by increasing the gap $\Delta_L$ and the potential $V$. The variation of $T_{KK}$ versus $\Delta_L$ is mainly contributed by the dominant reduction of $TKK$ for larger $\Delta_L$. It can be understood by the transport theory with single valley (see section Methods for detail). Meanwhile, the variation of $T_{KK}$ 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 $RKK^\prime$. Furthermore, the relationship of valley-polarization ratio $P$ versus potential $V$ for different $\Delta_L$ 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 $\Delta_L$. Such relationship is determined by the variation of $TKK^\prime$ versus $V$ and $T$. For fixed potential $V$, the band structure on the both sides of the junction becomes more asymmetrical by increasing of $\Delta_L$, leading to an enhancement of $TKK$. In contrast, by increasing $V$, $TKK^\prime$ 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 $\Delta_L$, the valley-polarization $P$ can be greatly improved with little expense of $T$. Inset of (f) is the schematic diagram for the carrier tunneling process.

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 $P$
decrease rapidly. From the relationship of $P$ versus $\Delta L$ 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 $V$.

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

$$V = E + \sqrt{E^2 + \Delta_R^2 - \Delta_L^2},$$

or

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

After the discovery of series of gapped valley materials recently\textsuperscript{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 $V$, $\Delta$ 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.

![Figure 7](image_url)

**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 $\Delta_R$. (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](image_url)

**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.
After 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 valleytron 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 $\Phi_{in}$ there are two reflection modes $\Phi_{r1}$, $\Phi_{r2}$ on the left side and two transmission modes $\Phi_{t1}$, $\Phi_{t2}$ on the right side. $\Phi_{in}$, $\Phi_{r1}$, $\Phi_{r2}$, $\Phi_{t1}$, $\Phi_{t2}$ on site $n$ are given by:

$$\Phi_{in}^n = \frac{h}{2\sqrt{4j_{L}A_{L}\cos{k_{L}}}} e^{ik_{L}n} \frac{1}{iA_{L}}$$

$$\Phi_{r1}^n = \frac{h}{2\sqrt{4j_{L}A_{L}\cos{k_{L}}}} e^{-ik_{L}n} \frac{1}{-iA_{L}}$$

$$\Phi_{r2}^n = \frac{h}{2\sqrt{4j_{R}A_{R}\cos{k_{R}}}} e^{ik_{R}n} \frac{1}{iA_{R}}$$

$$\Phi_{t1}^n = \frac{h}{2\sqrt{4j_{R}A_{R}\cos{k_{R}}}} e^{ik_{R}n} \frac{1}{-iA_{R}}$$

where $k_{L}$($k_{R}$) represents the wavevector of the mode $\Phi_{in}$($\Phi_{in}$) 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 $\Psi_{n}$ at site $n$ can be written as a combination of the incident modes and reflected/transmitted modes in the following equations:

$$\Psi_{n} = \begin{cases} \Phi_{in}^n + r_{1}\Phi_{r1}^n + r_{2}\Phi_{r2}^n, & n \leq 0; \\ t_{1}\Phi_{t1}^n + t_{2}\Phi_{t2}^n, & n \geq 1. \end{cases}$$

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

$$H_{0-}\Psi_{-1} + H_{in}\Psi_{0} + H_{t1}\Psi_{1} = E\Psi_{0},$$

$$H_{10}\Psi_{0} + H_{t1}\Psi_{1} + H_{t2}\Psi_{2} = E\Psi_{1}.$$
and its eigenfunction is $V$ and $JJ$. For simplicity, we focus on conduction band $(12)$. Consequently, we can get the corresponding transmission and reflection probabilities:

$$
t_1 = \frac{A_I (1 + e^{2ik_1})}{2x} \left[ \frac{1}{J \mathcal{A} e^{ik_1 + k_2} + A_L} \right] + \frac{1}{J A_I e^{i(k_2 + k_3)} + A_R} \right],
$$

$$
t_2 = \frac{A_I (1 + e^{2ik_1})}{2x} \left[ \frac{1}{J \mathcal{A} e^{ik_1 + k_2} + A_L} \right] - \frac{1}{J A_I e^{i(k_2 + k_3)} + A_R} \right],
$$

$$
r_1 = \frac{1 + e^{2ik_1}}{2} \left[ \frac{A_I}{J^{-1} A_L + JA_R e^{ik_1 + k_2}} - \frac{A_R}{J A_I e^{i(k_2 + k_3)} + A_R} \right],
$$

$$
r_2 = \frac{1 + e^{2ik_1}}{2} \left[ \frac{A_I}{J^{-1} A_L + JA_R e^{ik_1 + k_2}} + \frac{A_R}{J A_I e^{i(k_2 + k_3)} + A_R} \right] - 1,
$$

where $x = \sqrt{|A_I \cos k_1/(A_R \cos k_R)|}$ and $J = \sqrt{\left(1/(j_f j_k)\right)}$. Consequently, we can get the corresponding transmission and reflection probabilities:

$$
T_{KK} = |t_{1f}|^2, \quad T_{KK'} = |t_{2f}|^2,
$$

$$
R_{KK} = |r_{1f}|^2, \quad R_{KK'} = |r_{2f}|^2.
$$

$T_{KK}$ ($T_{KK'}$) 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

$$
T = T_{KK} + T_{KK'},
$$

and the valley polarization ratio

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

$T$ 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:

$$
H = \begin{bmatrix} V + \Delta & k \\ k & V - \Delta \end{bmatrix}.
$$

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

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

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

Finally, we obtain the reflection amplitude

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

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 $\Delta_R \to E - V$, the reflection amplitude $r \to 1$. It corresponds to the perfect reflection.

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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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