Transport properties of the electronic states in the gate voltage-modulated skyrmion crystal

Jianhua Gong and Rui Zhu

School of Physics and Optoelectronics, South China University of Technology, Guangzhou 510641, People’s Republic of China

Received 25 October 2021 / Accepted 17 January 2022 / Published online 3 February 2022
© The Author(s), under exclusive licence to EDP Sciences, SIF and Springer-Verlag GmbH Germany, part of Springer Nature 2022

Abstract. In this work, we investigated transport properties of the electronic states in the gate voltage-modulated skyrmion crystal (SkX). Dynamics of conducting electrons in the SkX can be described by the double-exchange model or the so-called \( t - J \) model, with the \( t \) term measuring the hopping energy of the electrons between neighboring sites and \( J \) term measuring the strength of the on-site Hund’s coupling between the spin of conducting electrons and local magnetization. As a result of the Hund’s coupling, the band structure of the conducting electrons in the SkX shares similar topological properties with that of gapped graphene, such as its cone-like shape, nonzero band Chern number, and edge states. By linear fitting the cone-shape energy dispersion of the electronic states in the SkX, one can obtain a gapped Dirac model similar to that of the gapped graphene. We use the Green’s function technique and calculate the transmission probability of the electrons tunneling through an electrostatic barrier in the SkX expressed by the double-exchange model. Numerical results of the transport properties of the SkX by the double-exchange model reproduced analytic results from the Dirac model. We further interpreted the resemblance between the transport properties of the two models by the likeness in their wave functions.

1 Introduction

Recently, magnetic states with nontrivial spin fields such as the magnetic domain walls [1,2] and magnetic bubbles with or without a skyrmion topology [3–11] have attracted great attention due to its potential spintronic application in race-track memory and logic gates. The magnetic skyrmion is the two-dimensional (2D) spin vortex texture bearing an integer topological number. Such a nontrivial spin field can originate from different mechanisms [3]. The most popular among these are the chiral materials with the Dzyaloshinskii-Moriya (DM) interaction [12,13] spiraling the spin, such as B20 compound MnSi, Fe\(_{1-x}\)Co\(_x\)Si, and single-layer Fe/Ir(111) [3,14–16]. Due to topological stability, it was demonstrated that the threshold current to drive a skyrmion to move is five orders smaller than that to drive a magnetic domain wall [6]. Writing and deleting of a magnetic skyrmion was realized demonstrating the potential application in information storage [5]. Magnetic skyrmion logic gates were predicted by numerical simulation [10].

Accompanying the exploitation of the nontrivial topology of the magnetic skyrmion in the real space, the nontrivial topology in the momentum space of the electronic states whirled by the background spin in the skyrmion crystal (SkX) also attracted a lot of interest. The SkX is periodically arranged magnetic skyrmions forming a square or triangular lattice. Most magnetic skyrmions discovered in the experiment exist in the state of the SkX. The electronic dynamics of the SkX can be described by a double-exchange model [17,18]. As a result of the strong Hund’s coupling, spin of the passing electrons tends to align to the direction of the local magnetization. This gives rise to a reassembled band structure of the electrons. Each band bears an integer Berry phase in the momentum space giving rise to a quantized intrinsic anomalous Hall conductivity, the so-called topological Hall effect [3,17,19,20,22,23]. The unique structure of magnetic skyrmion also produces topological spin Hall effect originated from the topological property of the Bloch bands [24], which is different from the physical mechanism of the spin Hall effect in the spin-orbit coupling system [25,26]. For opposite spins, the direction of the emergent electromagnetic field is opposite, so the opposite spins accumulated at the edge are deflected in the opposite direction. The flow direction of the spin depends on the edge-state spectrum. We mention the spin Hall effect because in our work of the single-barrier tunneling of the SkX when the energy of the incident electron matches the edge-state spectrum, the electrons will flow along the boundary of potential barrier and cannot pass through the potential barrier. Besides the topological Hall effect,
because the cone-like band structure is shared between the SkX and the multi-sublattice Dirac–Weyl materials such as graphene, Lieb lattice, and Dice lattice; other similar transport properties originally hosted by the Dirac family have been found in the SkX such as the topological phase transition driven by the next-nearest-neighbor hopping [27,28] and proximity-induced superconducting [29]. In the Dirac–Weyl fermionic family characterized by double-Dirac-cone dispersion, the Klein tunneling effect is theoretical predicted [30–34] and experimentally observed in graphene [35,36]. Naturally, one wonders if the transport properties of the conducting electrons in the SkX share similarities with that of the Dirac–Weyl fermionic family.

The difficulty lies in the technique. Non-equilibrium Green’s function (NEGF) is a very effective numerical method for calculating the transport behavior of nanoscale devices. It has been widely used to understand the transport properties of various materials and systems, such as organic molecules [37], graphene [38,39], silicon nanowires [40], and phonon transport [41]. Combining NEGF with the density functional theory and the tight-binding model investigation of computational materials becomes much more efficient [42,43]. The Green’s function approach bridging the tight-binding (TB) model and the effective Dirac equation has been proposed in the tunneling process of monolayer graphene [39]. By considering each skyrmion as a giant unit cell, we extend the TB calculation in graphene to the double-exchange model in the SkX. Surface Green’s function of the leads is calculated by the decimation method.

With the technique found, one motivation of the work is fulfilled, which is to pave way for a general numerical treatment of the transport property of multi-freedom crystal structures taking into account the background spin field and a complex unit cell. Recently, investigations in various systems have found that the transmission probability resembles as long as the energy dispersion has identical form regardless of the particular form of the Hamiltonian and its eigenvectors [39,44]. This encourages one to wonder whether the transport property of a complex Hamiltonian resembles the simple asymptotic Hamiltonian obtained by linear or parabolic band fitting. If so, one can predict the transport behavior of a complex system by its band structure in the low-energy regime if a rigorous calculation is beyond the current technique. This is the second motivation of the present work.

The relation between the transmission coefficient of single-barrier tunneling and the dispersion of the electronic states confined in the barrier-modulated nanoribbon has been demonstrated in various configurations of graphene, which is the origin of resonant tunneling [45–47]. In this work, we also investigated this relation of the electronic states in the single-barrier-modulated SkX. The NEGF and Dirac theory consistently recovered the relation between the transmission coefficient and the dispersion of the nanoribbon confined states. We also found the edge state flowing along the two sides of nanoribbon does not produce a transmission peak because their moving direction is perpendicular to the tunneling direction.

In addition, this work is not constricted in the adiabatic limit when the Hund’s coupling is extremely strong and the electronic spin completely aligns with the background magnetization. When the Hund’s coupling is reduced, the spin degree of the conducting electrons is partly set free, thus tunneling channel of different spins is redivurcated. The effect of weaker Hund’s coupling on the topological Hall conductivity was considered by various groups [48–51]. In this work, we numerically investigated the transmission coefficient of single-barrier tunneling when the Hund’s coupling strength changes from infinity to the magnitude of the hopping integral t. The transport behavior is qualitatively similar in this range, which is also the range that the topological Chern numbers of the electronic bands stays the same with those of the adiabatic limit [27].

The rest of this paper is organized as follows. Section 2 is attributed to the model and formalisms. In Sect. 2.1, we introduce the exchange model of describing the electronic dynamics of the SkX. In Sect. 2.2, we developed the non-equilibrium Green’s function technique (NEGF) for the TB model into the exchange model to investigate the electronic transport behavior of the SkX. As a parallel of the NEGF, in Sect. 2.2, we introduce the asymptotic Dirac model, which arises from the low-energy approximation of the electronic dispersion in the proximity of the Dirac cone apex. Analytic results of the transmission coefficient from the Dirac equation are also given in this subsection. In Sect. 3, numerical results of the transport properties of the SkX from the NEGF are given, which are compared with the asymptotic Dirac theory. Close consistency between the two models is demonstrated. In Sect. 4, a brief summary is presented.

2 Model and formalism

2.1 Double-exchange model in the skyrmion crystal

To simulate the transport properties of the SkX, we use the double-exchange model to describe the free electron system coupled with the background spin texture [17],

\[ H = \sum_i V_i c_i^\dagger c_i + t \sum_{i,j} c_i^\dagger c_j - J \sum_i n_i c_i^\dagger \sigma c_i, \]

where \( c_i = (c_i^\uparrow, c_i^\downarrow)^T \) is the two-component annihilation operator at the i site and \( c_i^\dagger \) is its creation counterpart. \( V_i \) correspond to the on-site potential at site \( i \) in the central region (see Fig. 1). \( t \) is the hopping integral between nearest-neighbor sites and \( J \) is Hund’s coupling strength between the electron spin and the background spin texture. \( n_i = (\cos \Phi_i \sin \Theta_i, \sin \Phi_i \sin \Theta_i, \cos \Theta_i) \) is the spin configuration in spherical coordinates. \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) indicates the vector of Pauli matrices.
In the strong-coupling limit, i.e., $J \gg t$, the spin of electron on site is forced to align parallel to the background spin texture. The effective hopping strength is determined by the spin overlap between neighboring sites $i$ and $j$, i.e., the effective hopping integral between nearest-neighbor sites is obtained by $\langle \chi_i | \chi_j \rangle$. The wave function $| \chi(r) \rangle$ of electron is the spin eigenstate of $n(r)$ at $r$. Using spherical coordinates in the spin space,

$$| \chi(r) \rangle = \left( \cos \frac{\Theta(r)}{2}, e^{i\Phi(r)} \sin \frac{\Theta(r)}{2} \right)^T, \quad (2)$$

and

$$t_{eff} = t \langle \chi_i | \chi_j \rangle = \cos \frac{\Theta_i}{2} \cos \frac{\Theta_j}{2} + \sin \frac{\Theta_i}{2} \sin \frac{\Theta_j}{2} e^{-i(\Phi_i - \Phi_j)}. \quad (3)$$

In this limit, the effective Hamiltonian reduces the degree of freedom of the spin [17]. Then,

$$H = \sum_i V_i d_i^\dagger d_i + \left( \sum_{i,j} t_{eff} d_i^\dagger d_j + \text{H.c.} \right). \quad (4)$$

Here, $d_i^\dagger$ is the spinless creation (annihilation) operator. $\theta_i$ and $\phi_i$ represent the polar and azimuthal angles on the $i$ site, respectively. The skyrmion profile is well assumed as $\Theta(r) = \pi (1 - r/\lambda)$ for $r < \lambda$ and $\Theta(r) = 0$ for $r > \lambda$, where $\lambda$ is radius of the skyrmion and $(r, \varphi)$ are the polar coordinates in the real space counting from the center of each skyrmion. When the skyrmion whirls in the pattern of $\Phi(\varphi) = \xi \varphi + \gamma$, the topological number is explicitly expressed by $Q = m \xi$ and $\gamma$ determines the helicity of the skyrmion. $\gamma = 0 (\pi/2)$ correspond to the Néel type and Bloch type skyrmions, respectively. The vorticity $m = \pm 1$ correspond to skyrmions and antiskyrmions, respectively.

We consider each skyrmion unit cell contains $5 \times 5 = 25$ atoms, setting the radius $\lambda = 2.5a$. $a$ is the atomic lattice constant. We construct an $npn$ junction shown in Fig. 1a or an $nn'n$ junction (in which the barrier is low and the Fermi level lies in the conduction band inside as well as outside the barrier) in the SkX. Due to the translation invariance in the transverse direction, we impose the Bloch theorem along the transverse direction with periodicity $W = 2\lambda = 5a$. Applying the boundary condition of period $W$, we modify the hopping strength between neighboring unit cells in the transverse direction by a Bloch phase factor $e^{\pm ik_y W}$.

Fig. 1 a Schematic image of the $npn$ junction of the Dirac theory with an energy gap. The blue filled areas indicate occupied states. The Fermi level lies in the conduction band in the left and right leads and in the valence band inside the barrier. The small picture above is the top view of the band showing the incident angle and the Fermi ring. b Schematic image of the $npn$ junction in the SkX consistent with that of panel (a). Shaded regions indicate the leads and the transparent region indicates the central barrier. The square made up of $5 \times 5$ circles indicates the minimum unit that simulates the bulk SkX with $W$ the transverse periodicity. The arrows describe the background spin of the SkX.
The process of recursive Green’s function. a The recursive process has not yet been carried out. b The first step in the recursive process. c The second step of the recursive process. d The last step of the recursive process shown in Fig. 1b. The whole system can be described by a one-dimensional chain. We get the relationship between the incident angle $\phi$ and $k_y$ on the Fermi ring, as shown in the upper part of Fig. 1a. It is worth noting that the shape of the Fermi ring is different for different Fermi energy. Figure 6 shows the Fermi ring of the lowest two bands of the SkX. If the selected Fermi energy is close to the peak of the Dirac cone, the Fermi ring here is basically a circle. We can use $k_y = \sin \phi k_f$ to calculate the angular dependence of the transmission probability.

The central region is finite in the transport direction. We perform the Fourier transform of the Hamiltonian along the $y$ direction. Then, the Fourier transform is written as $d_{mi} = \sum_{k_y} d_{k_y} e^{i k_y Y_{m}}$. The index “$m$” represents the position of the unit cell along the $x$ direction. By diagonalization of the Hamiltonian in the ribbon space, the energy spectrum as a function of the momentum $k_y$ is shown in Fig. 7a and c.

### 2.2 Non-equilibrium Green’s function

The Non-equilibrium Green’s function (NEGF) formalism provides a simple and effective method to describe the quantum transport at nanoscale [52]. Even so, there are so many atoms in the system that it makes our calculations difficult. By applying the Bloch’s theorem in the transverse direction [39,43], the system can be reduced to a one-dimensional chain. For a certain band energy $E$ and transverse wavevector $k_y$, we can numerically compute the retarded and advanced Green’s function as

$$G^r_{k_y}(E) = \left(G^a_{k_y}(E)\right)\dagger = \left((E + i\eta)I - H_{C,k_y} - \Sigma^r_{L,k_y} - \Sigma^r_{R,k_y}\right)^{-1}$$

Here, $\Sigma^r_{L} = H_{CL}g^L_{00}H_{LC}(\Sigma^r_{R} = H_{CR}g^R_{00}H_{RC})$ is the retarded self-energy of the left (right) lead. The surface Green’s function $g^L_{00}(g^R_{00})$ of the leads can be solved by the decimation method [53]. $H_C$ indicates the Hamiltonian for the central region. $H_{CL}/H_{CR}$ is the Hamiltonian connecting the central region and the left/right leads and $H_{LC}/H_{RC}$ is its Hermitian conjugate. $\eta$ and $I$ represent an infinitely small positive number and the identity matrix, respectively.

We calculate the transmission probability for an incident electron by the Fisher–Lee relation [54]

$$T(E, k_y) = \text{Tr}(\Gamma_L G^r \Gamma_R G^a),$$

$$G^r_{k_y}(E) = \left(G^a_{k_y}(E)\right)\dagger = \left((E + i\eta)I - H_{C,k_y} - \Sigma^r_{L,k_y} - \Sigma^r_{R,k_y}\right)^{-1}$$

Here, $\Sigma^r_{L} = H_{CL}g^L_{00}H_{LC}(\Sigma^r_{R} = H_{CR}g^R_{00}H_{RC})$ is the retarded self-energy of the left (right) lead. The surface Green’s function $g^L_{00}(g^R_{00})$ of the leads can be solved by the decimation method [53]. $H_C$ indicates the Hamiltonian for the central region. $H_{CL}/H_{CR}$ is the Hamiltonian connecting the central region and the left/right leads and $H_{LC}/H_{RC}$ is its Hermitian conjugate. $\eta$ and $I$ represent an infinitely small positive number and the identity matrix, respectively.

We calculate the transmission probability for an incident electron by the Fisher–Lee relation [54]
where the spectral functions was computed by \( \Gamma_{L/R} = i \left( \Sigma'_{L/R} - \Sigma''_{L/R} \right) \). When the Fermi energy \( E_f \) of the incident electron is determined, the correspondence between Bloch momentum \( k_f \) and the incident angle \( \phi \) is determined from the Fermi ring.

According to the Landauer–Büttiker formula, tunneling conductance of the electrons as a function of the Fermi energy can be expressed as

\[
G(E_f) = \frac{2e^2 W}{h} \int T(E_f, k_f)dk_f,
\]

where \( G_0 = \frac{e^2}{h} \).

It is time consuming to directly invert the large matrix at the right hand side of Eq (5) when the central region is large. We adopt the recursive Green’s function to avoid this problem [43,55,56], which is based on the Dyson equation. The central region is divided into slices, which only couple with neighboring slices as shown in Fig. 2a. Each slice is a single unit cell in the transport direction and extends to infinity in the transverse direction.

Numerically, we use a recursive process from left to right, or vice versa. At the first step, the Green’s function

\[
G^{(1)}_{11}(k_y) = (E - H_{11}(k_y) - \Sigma_{L}(k_y))^{-1}.
\]

The \( G^{(1)}_{11} \) means that the first slice is attached to the left lead shown in Fig. 2b. We repeat this procedure until the last slice \( N \),

\[
G^{(i)}_{ii}(k_y) = (E - H_{ii}(k_y) - \Sigma_{R}(k_y))\delta_{iN} - H_{i,i-1}G^{(i-1)}_{i,i-1}(k_y)H_{i-1,i}^{-1},
\]

\[
G^{(i)}_{ii}(k_y) = G^{(i-1)}_{i,i-1}(k_y)H_{i-1,i}(k_y)G^{(i-1)}_{ii}(k_y).
\]

When the first slice is attached to the left lead, a new lead surface is created, which is then attached to the second slice by a new surface Green’s function \( G^{(1)}_{11} \). The next step is that a new lead surface is attached to the third slice by a new surface Green’s function \( G^{(2)}_{22} \) until it is connected to the right lead. Through this recursive process, the entire central system has been taken into account. See Reference [43,55,56] for more details. Finally, the transport coefficient of the system can be obtained by

\[
T(E, k_y) = \text{Tr}(\Gamma_{L}G'_{1N}\Gamma_{R}G''_{1N}).
\]

### 2.3 Dirac theory

In the strong-coupling \( (J \gg t) \) limit, the structure of the lowest and second-lowest band has the properties of the Dirac cone. We can describe this electronic structure of massive Dirac fermions by the Dirac theory [17]

\[
H = \hbar v(-k_x \sigma_x + k_y \sigma_y) + m \sigma_z,
\]

where \( v \) is the Fermi velocity and the mass \( m \) is determined by the gap \( \Delta \) as \( m = \frac{\Delta}{2} \).

The eigenvalue of Eq. (12) is \( \lambda = \lambda \sqrt{v^2k^2 + m^2} \), \( \lambda = \pm 1 \) correspond to the conduction and valence bands, respectively. One assumes that the wave function of Eq. (12) is

\[
\psi_{\lambda,k} = \frac{1}{\sqrt{2}} \left( \psi(1) + \mu \lambda \right) e^{i(k_x x + k_y y)}.
\]

Putting the hypothetical wave function into Eq. (12), we get

\[
\psi_{\lambda,k} = \frac{1}{\sqrt{2}} \left( \begin{array}{c} \sqrt{1 + \frac{\lambda m}{\sqrt{m^2 + \hbar^2 v^2 k^2}}} - e^{-i\phi_k} \\ \pm \sqrt{1 - \frac{\lambda m}{\sqrt{m^2 + \hbar^2 v^2 k^2}}} \end{array} \right) e^{i(k_x x + k_y y)}.
\]

When the electron is incident into the square barrier \( V(x) = V_0(0 \leq x \leq D) \) shown in Fig. 1a. Then, the wave function in three different regions is

\[
\psi_i = \frac{1}{\sqrt{2}} \left( \begin{array}{c} \alpha e^{i(k_x x + k_y y)} \\ \mp \sqrt{1 + \frac{\lambda m}{\sqrt{m^2 + \hbar^2 v^2 k^2}}} - e^{-i\phi_k} \end{array} \right),
\]

\[
\psi_{ii} = \frac{1}{\sqrt{2}} \left( \begin{array}{c} \alpha e^{i(k_x x + k_y y)} \\ \mp \sqrt{1 - \frac{\lambda m}{\sqrt{m^2 + \hbar^2 v^2 k^2}}} \end{array} \right),
\]

\[
\psi_{iii} = \frac{1}{\sqrt{2}} \left( \begin{array}{c} \alpha e^{i(k_x x + k_y y)} \\ \mp \sqrt{1 + \frac{\lambda m}{\sqrt{m^2 + \hbar^2 v^2 k^2}}} \end{array} \right),
\]

\[
\begin{align*}
\alpha &= \sqrt{1 + \frac{\lambda m}{\sqrt{m^2 + \hbar^2 v^2 k^2}}}, \\
\gamma &= \sqrt{1 - \frac{\lambda m}{\sqrt{m^2 + \hbar^2 v^2 k^2}}}, \\
\beta &= \sqrt{1 + \frac{\lambda m}{\sqrt{m^2 + \hbar^2 v^2 k^2}}}, \\
\eta &= \sqrt{1 - \frac{\lambda m}{\sqrt{m^2 + \hbar^2 v^2 k^2}}}.
\end{align*}
\]

According to the continuity condition of the wave function, which is that the wave function is continuous at \( x = 0 \) and \( x = D \). Then,

\[
\begin{align*}
\alpha + r \alpha &= a \beta + b \beta, \\
-\lambda \gamma e^{-i\phi_k} + r \lambda \gamma e^{i\phi_k} &= -a \lambda \gamma e^{-i\phi_k} + b \lambda \gamma e^{i\phi_k}, \\
am \beta e^{i\phi_k} + b \beta e^{-i\phi_k} &= t \alpha e^{i\phi_k}, \\
-a \lambda' \gamma e^{-i\phi_k} e^{i\phi_k} + b \lambda' \gamma e^{i\phi_k} e^{-i\phi_k} &= -t \lambda \gamma e^{-i\phi_k} e^{i\phi_k}.
\end{align*}
\]
After some algebra, we can get transmission probability

\[ T = |t|^2 = \frac{\cos(\theta_q)^2 \cos(\phi_k)^2}{\sin(q_x D)^2 \left( \frac{N}{\lambda \lambda'} - 2 \sin(\phi_k) \sin(\theta_q) \right)^2 + (\cos(\phi_k) \cos(\theta_q) \cos(q_x D))}. \]  

(21)

In the transmission probability \( \frac{N}{\lambda \lambda'} = \frac{2 \lambda'}{\lambda} \left( \frac{|V_0 - E|}{\hbar^2 v^2 m^2} \right)^2 \), \( V_0 - E = \sqrt{m^2 + \hbar^2 v^2 q^2}, \ E = \sqrt{m^2 + \hbar^2 v^2 k^2}, \ q = \sqrt{k_y^2 + q_x^2}, \ k = \sqrt{k_y^2 + k_x^2}. \) The injection and refraction angles of the electron are \( \phi_k = \arctan(\frac{k_y}{k_x}) \) and \( \theta_q = \arctan(\frac{k_y}{q_x}) \), respectively.

For normal incidence, i.e., \( \phi_k = 0 \),

\[ T(\phi_k = 0) = \frac{1}{1 + \sin(q_x D)^2 \left( \left( \frac{N}{\lambda \lambda'} \right)^2 - 1 \right)}. \]  

(22)

Since \( \frac{N}{\lambda \lambda'} = \frac{2 \lambda'}{\lambda} \left( \frac{|V_0 - E|}{\hbar^2 v^2 m^2} \right)^2 \neq \pm 1 \), perfect transmission occurs when the condition \( q_x D = n\pi (n = 0, 1, 2, 3 \cdots) \) is satisfied.

3 Results and discussions

3.1 Transport behavior in the strong-coupling limit

In this section, we compare the tunneling results between the NEGF and the Dirac theory in the case of \( J \gg t \). In the NEGF treatment, we arbitrarily selected three Fermi energies of the incident electron: \( E_f = -3.1t, -3.08t, \) and \( -3.12t \) corresponding to \( E_f = 0.0825t, 0.1025t, \) and \( 0.0625t \) in Dirac theory, the latter of which is counted from the charge neutrality point. The width of the barrier is set to be \( D = 100 \) nm. To exactly match the barrier width, we set the lattice constant \( a = 1 \) nm in the double-exchange model. In this case, we can estimate the Fermi velocity from the SkX band to compare with the asymptotic Dirac theory by calculating the slope of the dispersion. Figure 3 show the transmission probability obtained from the NEGF and the Dirac theory, the two of which demonstrate close accordance. Figure 3b and the black curves in Fig. 3c demonstrate perfect transmission at normal incidence, which strongly confirms the occurrence of the Klein tunneling in the gate voltage-modulated SkX. We would like to remark here that the Klein tunneling is perfect transmission of the electronic states through the hole states. It can occur in gapped parabolic energy bands at normal incidence [57] and with massive pseudospin-1 particles [58]. The gap does not necessarily destroy the Klein tunneling. When the barrier is high enough to go over the gap and transmission of electrons is through hole states, Klein tunneling can occur. In addition, the NEGF and Dirac peaks at other incident angles, which results from resonance (electronic tunneling through vacuum states) or Klein tunneling (electronic tunneling through hole states when chirality of the quasiparticles is matched). We should note that there is still an angle difference of about \( 5^\circ \), which reflects the difference between the two methods, which was addressed in other systems [39].

Figure 3b demonstrates a difference between the two theories: there is one less transmission peak in the transmission probability obtained from the Dirac theory than that from the NEGF calculation. The reason is that the Dirac theory describes the linear dispersion relationship concerning low-energy excitation, which means that the Fermi ring in the energy space is

![Fig. 3](https://via.placeholder.com/150)

**Fig. 3** Transmission probability \( T(E_f, \phi) \) of the SkX obtained from the NEGF calculation and Eq. (21) of the Dirac theory. Solid and dashed lines are results of the NEGF and Dirac theory, respectively. In panels a and b, \( E_f = -3.1t, V_0 = 0.15t \) and \( 0.2t \), respectively. In panels c and d, \( E_f = -3.08t \) and \( -3.12t \), respectively.
Fig. 4 Transmission probability as a function of barrier height $V_0$ at normal incidence. a and b Are calculated from the Dirac theory and the NEGF, respectively. The Fermi energy of the incident electron is $E_f = -3.1t$ for NEGF. c Represents the Fermi energy position corresponding to the height of the central barrier.

In the Dirac theory, it is predicted that the transmission peak will appear on $q_x D = n\pi$ at normal incidence. We keep the width $D$ of the barrier constant and change the height $V_0$ of the barrier to modify $q_x$ by $q_x = \sqrt{\frac{(V_0-E)^2 - m^2}{\hbar^2 v^2}}$. Results of the calculation is shown in Fig. 4a. Since $q_x$ is not involved in the NEGF calculation, we only need to modify $V_0$ in the Hamiltonian of the central region. The corresponding results are shown in Fig. 4b.

When the height of the barrier $V_0 \leq 0.0514t$, the incident electron travels from the conduction band at the left lead through the conduction band at the barrier and finally reaches the conduction band at the right lead, which is an $nn'$ junction. When the barrier goes up to $0.0514t \leq V_0 \leq 0.1136t$, the Fermi energy of circular. But a real Fermi ring of the electronic states in the SkX is not a circle, which means that the Fermi velocity and $q_x$ are not fixed. We can get this information from the band structure. Since the small difference in the incident angle obtained from the two theories, the missing transmission peak has gone beyond $90^\circ$ and is therefore missing.

In the Dirac theory, it is predicted that the transmission peak will appear on $q_x D = n\pi$ at normal incidence. We keep the width $D$ of the barrier constant and change the height $V_0$ of the barrier to modify $q_x$ by $q_x = \sqrt{\frac{(V_0-E)^2 - m^2}{\hbar^2 v^2}}$. Results of the calculation is shown in Fig. 4a. Since $q_x$ is not involved in the NEGF calculation, we only need to modify $V_0$ in the Hamiltonian of the central region. The corresponding results are shown in Fig. 4b.

When the height of the barrier $V_0 \leq 0.0514t$, the incident electron travels from the conduction band at the left lead through the conduction band at the barrier and finally reaches the conduction band at the right lead, which is an $nn'$ junction. When the barrier goes up to $0.0514t \leq V_0 \leq 0.1136t$, the Fermi energy of

Fig. 5 Real component of the real-space wave function of the two cone-shape energy bands contributing to the transport behavior in the Skyrmion crystal (a, b) and in the Dirac theory obtained by lineal fitting the lowest two bands of the SkX (c, d). Panels a and c are results of the lower cone band and panels b and d are results of the upper cone band. We use color hue to express the magnitude of the wave function normalized to its maximal value within the real-space view window ($x \in [0,50a]$ and $y \in [0,50a]$ for the SkX and $x \in [0,75a]$ and $y \in [0,75a]$ for the Dirac theory). Inset is the color bar used. For all the subfigures a unit cell of size $5a \times 5a$ is considered. We calculated the wave function of the lattice model in the SkX. There are $5 \times 5 = 25$ atoms in each unit cell of the SkX and each atom is represented by a colored dot in the figure. For the Dirac theory, we assumed a two-sublattice model in which each row of the spinor wave function corresponds to one sublattice. Each assumed “atom” is represented by a colored rectangular in the figure. For all the subfigures $k_x = k_y = 0.04\pi$. Other parameters are the same to Figs. 3.
the incident electron is in the energy gap of the barrier region. Since neither the electron nor the hole state fills the gap, the incident electron lacks resonant level at the barrier and crossing of the electron is prevented. The transmission probability is zero disregarding whether we use the Dirac theory or the NEGF. As the barrier rises further, the Fermi energy locates in the valence band in the barrier region. The electron transport turns into hole transport in the valence band and finally turns back into electron transport in the conduction band in the right lead, giving rise to the Klein tunneling effect. This is an *npn* junction. If we lifted the central barrier even higher, the Fermi energy exceeds the Dirac cone band range, no transmission occurs, which is the same as in the band gap.

In the case of low-energy excitation, the transmission property obtained by Dirac theory is consistent with the NEGF. In the case of high energy excitation, nonlinear effect of the band is obvious and the Dirac theory is no longer applicable. Nevertheless the NEGF method can be applied at any energy.

To interpret the resemblance of the transport behavior between the SkX of the lowest two cone-shape bands and the Dirac theory obtained from linear fitting the two bands, we sampled one state from each cone band and calculated the real-space wave function of the two model. Wave function of the SkX can be obtained from the eigen-spinors of Hamiltonian (4) and wave function of the corresponding Dirac model is given in (13). The results are shown in Fig. 6. We chose a wave vector \( kx=ky=0.04 \pi \) close to the cone apex for both models where the bands and the transmission probabilities show likeness between the two models. For the Dirac theory, we assumed a two-sublattice model in which each row of the spinor wave function corresponds to one sublattice. From the figure, we can see that although the wave functions are not exactly the same, rough large-scale resemblance is evident. If you half close your eye into a slim line you can see that in both (a) (c) warm–color wider regions are divided by cold–color ridges and the ridges are in the same spatial location for the two panels (note the size difference between the two panel) and in both (b) and (d) red or pink color belts are prominent in the square space and locate in the same position. In the figure, warm color corresponds to larger magnitude of the wave function and cold color to smaller magnitude of the wave function (see the color bar). Therefore the wave function demonstrates periodic and strength likeness between the two models hence it lends us a more profound interpretation of the transmission likeness between the two models. And the transmission coefficients of the two models shown in Figs. 4 and 5 are not exactly the same, so that any difference between the wave function of the two models concordantly exists.

### 3.2 Transmission probability of finite Hund’s coupling

In this section, we analyze transmission probability in the case of finite Hund’s coupling. In this case, influence of the electron spin subjected to the background spin texture is limited. We have to take into account the two spin directions of the electron. A transmission probability of 2 means that electrons in both spin directions can cross the barrier completely. Since the range of the energy bands is different under different Hund’s coupling strength \( J \). As a result of the finite Hund’s coupling, the position of the energy bands changes a little in comparison with the case of the infinite Hund’s coupling. To compare the two cases and to see a strong Klein tunneling effect, we tune the Fermi energy and the barrier height according to the band structure for different Hund’s coupling strength to have the Fermi energy 0.02 higher than the conduction bottom in the leads and simultaneously 0.02 lower than the valence band top in the barrier. In this way, filling pattern of the electrons in the leads and that of the holes in the barrier is the same.

In Fig. 5a, when \( J < 1.3t \), the transport coefficient exceeds 1 because of the electron spin is not aligned with the background SkX and the spin degree of freedom is taken into account. When \( J \geq 1.3t \), the electron spin effect disappeared, which shows that the Hund’s coupling strength is sufficient to restrain the direction of electron spin deflection. As the coupling strength increases, the shape of the transport probability \( T \) gradually changes to that obtained in the strong coupling limit by comparison of Figs. 3 and 5b.

### 3.3 Transmission probability and band

We analyze the relationship between the transmission probability and the band configuration by concerning
Fig. 7  

The bands described by the Dirac equation (12) and e the lowest two bands described by the effective tight-binding model of the SkX under the strong coupling condition \( J \gg t \). The corresponding energies of Fermi cross profile a–c are \( E_f = -3.0438t \), \( E_f = -3.3t \) and \( E_f = -3.55t \).

Fig. 8  

a and c Transmission probability as a function of the incident angle \( \phi \) and the barrier height \( V_0 \). b and d Band structure of the central nanoribbon (the central barrier region can be looked at as a nanoribbon along the transverse direction of the transport). In b and d, blue and green curves correspond to the edge states flowing perpendicular to the tunneling direction, which do not contribute to the transmission (see Fig. 9). Barrier widths \( D = 20 \) skyrmions (one skyrmion constitutes one slice in the NEGF treatment) for (a), (b) and 10 skyrmions for (c), (d), respectively. The Fermi energy is set to be \( E_f = -3.1t \) in the edge states. In this part, we mainly discuss the situation of \( J \gg t \), where the Dirac cone of the SkX is easier to observe as shown in Fig. 6d. Gradually increasing the barrier height in the central region can change the band position of the central region where the Fermi energy is aligned. The Fermi energy of \( E_f = -3.1t \) in the left lead aligns with the energy of \( E = -3.3t \) in the valence band of the central region when the barrier height is \( V_0 = 0.2t \), where the cross profile belongs to the Dirac cone energy shown in Fig. 6b. The boundary of the Dirac cone is shown in Fig. 6a, where results of the NEGF began to deviate from the Dirac theory. The outside of the Dirac cone cannot contribute to trans-
Fig. 9  a Transmission probability as a function of the incident angle $\phi$ and the barrier height $V_0$. b Energy bands of the nanoribbon in the central region. In (b), blue and green curves correspond to the edge states flowing perpendicular to the tunneling direction, which do not contribute to the transmission (see Fig. 9). $D = 10$ slices and $E_f = -3.044t$.

Fig. 10  The sketch illustrates why the edge states do not contribute to the transmission coefficient shown in Figs. 7 and 8. The blue and green curves correspond to the spin-down and spin-up electrons, respectively. The red curves correspond to tunneling of the bulk electronic states. Properties of these edge states were demonstrated in the topological spin Hall effect of the magnetic skyrmions in Ref. [24].

Fig. 11  Change in conductance with taking into account potential barrier. The Fermi energy of the incident electron is $E_f = 3.1t$. The red line and the black line correspond to 10 slices and 20 slices in the central region, respectively.

Calculating transmission probability as a function of the incident angle $\phi$ and the barrier height $V_0$ at $E_f = -3.1t$ can capture three pieces of information. First, total reflection appears inside the band gap and outside of the Dirac cone in the central region. Second, the number of lines with a transmission coefficient of 1 for the npn junction is the same as the number of the valence band line of the nanoribbon geometry. Figure 7b shows that the valence band line of the nanoribbon geometry with a barrier width of 20 slices is only 19, because that the missing line is the edge state inside the gap. It is interesting that the line of the transmission coefficient of 1 for the npn junction is also 19 as shown in Fig. 7a. The same phenomenon also occurs in the case of $D = 10$ slices shown in Fig. 7c and d. This demonstrates that tunneling of the electron occurs through the eigenstates of the middle barrier. When the energy of the incident electron matches the edge-state spectrum, the electrons will flow along the boundary of potential barrier and cannot pass through the potential barrier, which is illustrated in Fig. 9. Third, besides the number of the perfect transmission peaks, the sparse and dense positions of the two are basically the same. The relation between the transport property and the band structure of the material is further confirmed.

The same situation occurs with nn'n junction. But it is difficult to observe how many lines with a transmission coefficient of 1 there are, because the lines above are too dense to merge together as shown in Fig. 8a. The large red part in the upper half of the figure is the transmission probability of the nn'n junction, in which the incident level aligned with one level in the conduction band of the central region. The bottom half of the figure is the npn junction, in which the incident level aligned with one level in the valence band of the central region. It is again shown that the transmission characteristics coincide with the dispersion of the quasiparticle eigenstates of the central nanoribbon.

In the end, by calculating the conductance $G$, we find that the conductance of the nn'n junction is close to a linear reduction corresponding to the linear reduction
of the density of states of the conduction band as the barrier increases, which can be interpreted by the upper half red-color region in Fig. 8a. For the npn junction, discrete levels in the valence band give rise to oscillation in the conductance, which can be interpreted by Fig. 8b.

4 Conclusions

In this work, we use the NEGF method and the Dirac theory to analyze the transport property of the electron states in the gate voltage modulated SkX. The infinite and finite Hund’s coupling conditions are taken into account. The angular dependence of the transmission probability is obtained and close consistency between the two methods in the adiabatic is demonstrated. By developing the TB NEGF to the exchange model, transport properties of the SkX with finite Hund’s coupling are obtained. For small Hund’s coupling, the transmission coefficient exceeds 1 because the Hund’s coupling is strong enough to restrain the electron spin along the background SkX spin field. By comparing the contour of the transmission probability in the space and the band structure of the nanoribbon geometry in the central barrier region, we show that the energy band of the central region is reflected in the transmission probability, which demonstrates resonant tunneling. Therefore, the transport properties of the electronic states in the gate voltage-modulated SkX are similar to those of gapped graphene, which can be well approximated by the Dirac model obtained from linear fitting the energy dispersion of the SkX Figs. 10, 11.

Acknowledgements R.Z. is grateful for enlightening discussions with Pak Ming Hui. We acknowledge support by the National Natural Science Foundation of China (No. 11004063) and the Fundamental Research Funds for the Central Universities, SCUT (No. 2017ZD099).

Author contributions

Both the authors contributed equally to this study.

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors’ comment: All data included in this manuscript are available upon request by contacting with the corresponding author.]

References

1. K.-S. Ryu, L. Thomas, S.-H. Yang, S.P. Chiral, Nat. Nanotechnol. 8, 527 (2013)
2. R. Zhu, J. Berakdar, Phys. Rev. B 81, 014403 (2010)
3. N. Nagaosa, Y. Tokura, Nat. Nanotechnol. 8, 899 (2013)
4. S. Mühlbauer, B. Binz, F. Jonietz, C. Pfleiderer, A. Rosch, A. Neubauer, R. Georgii, P. Böni, Science 323, 915 (2009)
5. N. Romming, C. Hanneken, M. Menzel, J.E. Bickel, B. Wolter, K.V. Bergmann, A. Kubetzka, R. Wiesendanger, Science 341, 636 (2013)
6. F. Jonietz, S. Mühlbauer, C. Pfleiderer, A. Neubauer, W. Münzer, A. Bauer, T. Adams, R. Georgii, P. Böni, R.A. Duine, K. Everschor, M. Garst, A. Rosch, Science 330, 1648 (2010)
7. Y. Su, S. Hayami, S.Z. Lin, Phys. Rev. Res. 2, 013160 (2020)
8. S. Hayami, Y. Motome, Phys. Rev. B 99, 094420 (2019)
9. R. Ozawa, S. Hayami, Y. Motome, Phys. Rev. Lett. 118, 147205 (2017)
10. X. Zhang, M. Ezawa, Y. Zhou, Sci. Rep. 5, 9400 (2015)
11. P. Zhang, A. Das, E. Barts, M. Azhar, L. Si, K. Held, M. Mostovoy, T. Banerjee, Phys. Rev. Res. 2, 032006(R) (2020)
12. I. Dzyaloshinsky, J. Phys. Chem. Solids 4, 241 (1958)
13. T. Moriya, Phys. Rev. 120, 91 (1966)
14. S. Heinze, K.V. Bergmann, M. Menzel, J. Brede, A. Kubetzka, R. Wiesendanger, G. Bihlmayer, S. Blügel, Nat. Phys. 7, 713 (2011)
15. S. Seki, X.Z. Yu, S. Ishiwata, Y. Tokura, Science 336, 198 (2012)
16. T. Tanigaki, K. Shibata, N. Kanazawa, X. Yu, Y. Onose, H.S. Park, D. Shindo, Y. Tokura, Nano Lett. 15, 5438 (2015)
17. K. Hamamoto, M. Ezawa, N. Nagaosa, Phys. Rev. B 92, 115417 (2015)
18. M. Onoda, G. Tataru, N. Nagaosa, J. Phys. Soc. Jpn. 73, 2624 (2004)
19. A. Neubauer, C. Pfleiderer, B. Binz, A. Rosch, R. Ritz, P.G. Niklowitz, P. Böni, Phys. Rev. Lett. 102, 186602 (2009)
20. S.X. Huang, C.L. Chien, Phys. Rev. Lett. 108, 267201 (2012)
21. N. Kanazawa, Y. Onose, T. Arima, D. Okuyama, K. Okoyama, S. Wakimoto, K. Kakurai, S. Ishiwata, Y. Tokura, Phys. Rev. Lett. 106, 156603 (2011)
22. B. Göbel, A. Mook, J. Henk, I. Mertig, Phys. Rev. B 95, 094413 (2017)
23. B. Göbel, A. Mook, J. Henk, I. Mertig, Phys. Rev. B 96, 060406(R) (2017)
24. G. Yin, Y. Liu, Y. Barlas, J. Zang, R.K. Lake, Phys. Rev. B 92, 024411 (2015)
25. C.L. Kane, E.J. Mele, Phys. Rev. Lett. 95, 226801 (2005)
26. X.-L. Qi, Y.-S. Wu, S.-C. Zhang, Phys. Rev. B 74, 085308 (2006)
27. J. Gong, R. Zhu, Phys. Lett. A 390, 205 (2021)
28. W. Beugeling, J.C. Everts, C.M. Smith, Phys. Rev. B 86, 195129 (2012)
29. A. Kubetzka, J.M. Burger, R. Wiesendanger, K.V. Bergmann, Phys. Rev. Mater. 4, 081401(R) (2020)
30. M.I. Katsnelson, K.S. Novoselov, A.K. Geim, Nat. Phys. 2, 620 (2006)
31. P.E. Allain, J.N. Fuchs, Eur. Phys. J. B 83, 301 (2011)
32. E. Illes, E.J. Nicol, Phys. Rev. B 95, 235432 (2017)
33. R. Shen, L.B. Shao, B. Wang, D.Y. Xing, Phys. Rev. B 81, 041410(R) (2010)
34. A. Fang, Z.Q. Zhang, Steven G. Louie, C.T. Chan, Phys. Rev. B 93, 035422 (2016)
35. A.F. Young, P. Kim, Nat. Phys. 5, 222 (2009)
36. N. Stander, B. Huard, D. Goldhaber-Gordon, Phys. Rev. Lett. 102, 026807 (2009)
37. P.S. Damle, A.W. Ghosh, S. Datta, Phys. Rev. B 64, 201403 (2001)
38. R.N. Sajjad, S. Sutar, J.U. Lee, A.W. Ghosh, Phys. Rev. B 86, 155412 (2012)
39. M.-H. Liu, J. Bundesmann, K. Richter, Phys. Rev. B 85, 085406 (2012)
40. J. Wang, E. Polizzi, M. Lundstrom, J. Appl. Phys. 96, 2192 (2004)
41. N. Mingo, L. Yang, Phys. Rev. B 68, 245406 (2003)
42. J. Taylor, H. Guo, J. Wang, Phys. Rev. B 63, 245407 (2001)
43. R.N. Sajjad, C. Polanco, A.W. Ghosh, J. Comput. Electron. 12, 232 (2013)
44. M. Wimmer, Ph.D. thesis, Universität Regensburg, 2008
45. J.M. Pereira Jr., V. Mlinar, F.M. Peeters, P. Vasilopoulos, Phys. Rev. B 74, 045424 (2006)
46. A. Iurov, L. Zhemchuzhna, P. Fekete, G. Gumbs, D. Huang, Phys. Rev. Res. 2, 043245 (2020)
47. F. Anwar, A. Iurov, D. Huang, G. Gumbs, A. Sharma, Phys. Rev. B 101, 115424 (2020)
48. K.S. Denisov, I.V. Rozhansky, N.S. Averkiev, E. Lähderanta, Sci. Rep. 7, 17204 (2017)
49. K.S. Denisov, I.V. Rozhansky, N.S. Averkiev, E. Lähderanta, Phys. Rev. B 98, 195439 (2018)
50. K. Nakazawa, M. Bibes, H. Kohno, J. Phys. Soc. Jpn. 87, 033705 (2018)
51. K. Nakazawa, H. Kohno, Phys. Rev. B 99, 174425 (2019)
52. S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, 1995)
53. M.P. LopezSancho, J.M. LopezSancho, J. Rubio, J. Phys. F 15, 851 (1985)
54. D.S. Fisher, P.A. Lee, Phys. Rev. B 23, 6851 (1981)
55. C.H. Lewenkopf, E.R. Mucciolo, J. Comput. Electron. 12, 203 (2013)
56. D. Ryndyk, *Theory of Quantum Transport at Nanoscale* (Springer, New York, 2016)
57. R. Du, M.-H. Liu, J. Mohrmann, F. Wu, R. Krupke, H.V. Lohneysen, K. Richter, R. Danneau, Phys. Rev. Lett. 121, 127706 (2018)
58. Y. Betancur-Ocampo, G. Cordourier-Maruri, V. Gupta, R. de Coss, Phys. Rev. B 96, 024304 (2017)