Geometrical spin manipulation in Dirac flakes

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Abstract
We investigate numerically the spin properties of electrons in flakes made of materials described by the Dirac equation, in the presence of intrinsic spin–orbit coupling (SOC). We show that electrons flowing along the borders of flakes via edge states become helically spin-polarized for strong SOC, for materials with and without a gap at the Fermi energy, corresponding to the massive and massless Dirac equation respectively. The helically spin-polarized electrons create spin-resolved transport, controlled by the flake’s geometry in a multi-terminal device setup. A simple analytical model containing the basic ingredients of the problem is introduced to get an insight into the helical mechanism, along with our numerical results which are based on an effective tight-binding model.

Keywords: Dirac materials, quantum transport, spin–orbit coupling, edge states

1. Introduction
Mesoscopic low-dimensional materials described by the Dirac equation are a rapid developing field, providing a vast area for fundamental research and promising a wide range of applications. One of the earliest examples is graphene, a two-dimensional (2D) sheet of carbon atoms arranged in a honeycomb lattice structure, resulting in an electronic behavior at the Fermi level that resembles relativistic massless particles described by the massless Dirac equation [1, 2]. Another, more recent example is transition metal dichalcogenide (TMD) monolayers [3–11], with a honeycomb lattice structure similar to graphene but with a large gap at the Fermi level, for instance 1.83 eV for MoS₂. Alternatively, a gap could be created in graphene by placing it on top of boron nitride (BN) substrates [12–15]. Graphene on BN substrates and TMD monolayers can be effectively described by the massive Dirac equation, instead of the massless one that describes pristine graphene.

Dirac materials can be easily formed in confined dot-like structures of various sizes and shapes, known as flakes, and have been studied theoretically and demonstrated experimentally [1, 16–27]. Specifically for TMD flakes, the trigonal shape is a natural state in their experimental preparation [26, 27]. The confinement in Dirac flakes leads to unconventional electronic properties such as edge states, whose electronic density is concentrated at the border of the flakes [17–19, 28], leading to novel topological phenomena [29–32]. Edge states are fundamentally a consequence of quantum interference in the honeycomb lattice structure present in Dirac materials.

On the other hand, spin–orbit coupling (SOC) in Dirac materials offers the possibility to manipulate the electron spin for integration in spintronic applications [33–36]. Despite the weak SOC in graphene, the interaction with the system’s confinement, particularly in graphene nanoribbons, has been shown to produce novel quantum phases like the quantum-spin-Hall (QSH) phase [37–40]. The QSH effect has sparked a growing interest in exotic materials that display related behaviors, known as topological insulators. Also, spin-transport effects have been investigated in graphene flakes via DFT simulation [41, 42]. In the same sense, TMD monolayers and other emergent 2D materials are also promising candidates for relevant theoretical investigations [43] and applications since the SOC strength can be much higher than graphene, leading to large spin splittings of up to 0.46 eV in some cases of TMD monolayers [44].
In the current work we analyze the spin properties of electrons in Dirac flakes with intrinsic SOC via the numerical calculation of the transmission probabilities along the border of the flakes. We show that, for sufficiently strong SOC, electrons that propagate in opposite directions along the flake’s border via the edge states have opposite spins, leading to helically spin-polarized electrons. We demonstrate this property in a multi-terminal device setup naturally formed by attaching three leads at the corners of a trigonal flake. Appropriate tuning of the chemical potential of the leads creates spin-resolved electronic transport via the different sides of the triangle, leading to spin-polarized currents, controlled by the flake’s geometry. This allows a geometrical manipulation of the spin intrinsically without the need to apply external fields. The helically spin-polarized electrons are present in materials with and without a gap at the Fermi energy, described by the massive and massless Dirac equation respectively, which could correspond to TMD monolayers and graphene. Additionally, we introduce a simplified analytical model that contains the fundamental ingredients of the numerical model, allowing us to get a better understanding of our numerical results.

2. Model

In this section, we present our numerical tight-binding model to simulate flakes made out of Dirac materials in the presence of SOC. Dirac materials can be described by the massive Dirac equation [43, 45–50] with Hamiltonian

\[ H_0 = \frac{\hbar v_F}{2} (\sigma_x \partial_x + \sigma_y \partial_y) + V \sigma_3 \]  

(1)

where $v_F$ is the Fermi velocity of electrons, whose value depends on the material under investigation, and $\sigma_i$ are the Pauli matrices acting on orbital space. The symbol $\tau_z = \pm 1$ denotes the non-equivalent valleys that are present in graphene and other Dirac materials like TMD monolayers, at the six corners of their hexagonal Brillouin zone. Different values of $V$ classify different materials; for example, $V = 0$ meV corresponds to graphene, while finite $V$ could describe TMD monolayers and graphene on BN substrates [15, 43, 45–47].

In order to perform our numerical calculations, we consider an effective tight-binding model, consisting of a honeycomb lattice with first-nearest-neighbor hopping, along with an on-site staggered potential simulating the mass term in equation (1),

\[ H_0 = \sum_{\langle i,j \rangle, \mu} t_{ij} (c^\dagger_{i\mu} c_{j\mu} + c^\dagger_{j\mu} c_{i\mu}) + \sum_i \epsilon_i c^\dagger_{i\uparrow} c_{i\downarrow} + \sum_i V_i c^\dagger_{i\uparrow} c_{i\downarrow}, \]  

(2)

where $c^\dagger_{i\mu}$ ($c_{i\mu}$) is the creation (annihilation) operator for spin $\mu$ at site $i$ while $t_{ij} = 1$eV is a uniform hopping between all the nearest-neighbor lattice sites. The on-site potential $\epsilon_i$ is $V$ and $-V$ on A and B sublattice sites respectively, with $V = 0$ corresponding to graphene. The staggered potential breaks the inversion symmetry, opening a gap $2V$ at the Fermi energy for infinite unbounded systems. At low energies the effective tight-binding Hamiltonian equation (2) transforms to equation (1) with $\hbar v_F = \frac{\epsilon i}{\tau_z}$ where $a$ is the lattice constant. This effective tight-binding model can be thought of as a numerical version of the massive Dirac equation.

The SOC can be introduced in the tight-binding model by considering spin-dependent between next-nearest neighbors in the honeycomb lattice as [37, 46],

\[ H_{SOC} = i\alpha \sum_{\langle\langle i,j \rangle, \mu, \mu' \rangle} \nu_{ij} c^\dagger_{i\mu} \sigma_\alpha c_{j\mu'}, \]  

(3)
where $S$ is the Pauli matrix while the sum runs over next-nearest neighbors on both sublattices. We consider spin-dependent amplitude $\eta_{ij} = +1 (-1)$ if an anticlockwise (clockwise) turn is required to move from site $i$ to its second-nearest-neighbor site $j$ via its first-nearest-neighbor, represented by curved arrows inside the honeycomb lattice of the trigonal flake in figure 1. The strength of the intrinsic SOC is determined by $\alpha$. We note that the SOC interaction described by equation (3) involves connections between sites belonging to the same sublattices A or B, in conjunction with the first-nearest-neighbor term in equation (2), which involves connections only between A and B sublattice sites. Equation (3) is responsible for the QSH effect in confined graphene systems, acting as a bridge between graphene and topological insulators. The total Hamiltonian of our system is

$$H = H_0 + H_{\text{SOC}}.$$  \hspace{1cm} (4)

By applying hard-wall boundary conditions to equation (4) we can simulate trigonal flake like the one shown in figure 1. We characterize the flake size by the length of the triangle’s base $L$ in units of the lattice constant $a$.

In order to calculate the transmission probabilities via the edges of the trigonal flake, we attach perfect semi-infinite linear chains at the three A-type sites at the corners of the flake via hopping $t = 1$ eV, thus forming a three-terminal device, as shown in figure 1. The linear chains are described by $H_{\text{1D}} = \sum_{i,j} \left( t_{ij}^a c_{i,j}^\dagger c_{i,j} + t_{ij}^b c_{i+1,j}^\dagger c_{i,j} + t_{ij}^c c_{i,j}^\dagger c_{i-1,j} \right)$ where for simplicity we consider the same hopping $t$ inside the lead. The energy $E$, the SOC strength $\alpha$ and $V$ are all reported in units of $t$.

We observe that equation (3) contains only $\eta$, so that the total Hamiltonian of the system equation (4) can be split into spin-up and spin-down diagonal blocks, resulting in zero transmission probability between opposite spins (see appendix A). Therefore the transmission probability from lead $i$ to lead $j$ can be written as $T_{ij}^{\mu} = |\langle \Psi_\mu_{kj} | \Psi_{\mu_{ij}} \rangle|^2$, which can be used to estimate the degree of spin polarization. $T_{ij}^{\mu}$ can be calculated by using the appropriate Green’s function element corresponding to an excitation from a corner site in the flake where lead $i$ is connected, giving a response at another corner site where lead $j$ is connected. This element is $G_{ij}^{\mu}(E) = \left[ (E^\dagger - H^\mu - \Sigma_1(E) - \Sigma_2(E) - \Sigma_3(E) + \Sigma_3(E))^\dagger \right]_{ij}$, with $E^\dagger = e + i\eta$ where $E$ is the incident energy with $\eta \to 0^+$, while $\Sigma_3(E)$ is the self-energy of each semi-infinite linear chain. We consider two independent modes carrying spin up and spin down, for each left- and right-moving channel in the leads, giving the respective self-energies, since for 1D systems we can neglect the SOC (see appendix A). By using the group velocity in the leads and applying the Fisher–Lee relations for transport [51] we get $T_{ij}^{\mu}(E) = (4 - E^2) |G_{ij}^{\mu}(E)|^2$.

3. Edge states

In this section, we analyze the edge states present in trigonal zig-zag flakes made of Dirac materials, which are responsible for the electronic behavior near the Fermi level. Edge states in graphene nanoribbons with staggered potential have been investigated in [52]. In the lattice representation, the number of edge states can be derived by algebraic arguments applied on the honeycomb lattice, which is bipartite [53]. In general the Dirac flakes can be split into two sublattices where $N_A$ and $N_B$ are the respective numbers of A and B sublattice sites, as shown in figure 1. The type of the outermost atoms at the zig-zag edges of the flake determines which number is larger, $N_A$ or $N_B$. For the configuration in figure 1, we have $N_B > N_A$. While $N_B - N_A = L - 1$. We note that the type of atoms A and B can be easily changed by changing the orientation of the flake’s base on an infinite graphene sheet by 60°, compared to the base of the flake in figure 1, resulting in $N_A > N_B$ in this case. Since the spin–orbit coupling given by equation (3) contains only $\eta$, it does not mix the spin-up and the spin-down orientations, so that the total Hamiltonian of the system can always be split into spin-up and spin-down diagonal blocks. Consequently we can write down the Schrödinger difference equations centered on atoms A and B for spin-up(down) denoted by $\mu = (1,-1)$ as

$$\begin{align*}
(E - \epsilon_A) \Psi_{\mu_{A,i}} &= t \sum_j \Psi_{\mu_{B,j}}^\dagger + \eta \alpha \sum_j \nu_\mu \Psi_{\mu_{A,j}} \\
(E - \epsilon_B) \Psi_{\mu_{B,i}} &= t \sum_j \Psi_{\mu_{A,j}}^\dagger + \eta \alpha \sum_j \nu_\mu \Psi_{\mu_{B,j}} 
\end{align*}$$  \hspace{1cm} (5)

where $\Psi_{\mu_{A,B}}$ is the wavefunction amplitude on site $i$ of each sublattice with spin $\mu$ and $\epsilon_{A,B}$ is the staggered on-site potential on sublattice A(B). In both sets of equations, the first term on the right-hand side comes from the nearest-neighbor hopping, while the second term is associated with the second-nearest-neighbor hopping with spin-dependent amplitude $\nu_\mu$, as in equation (3). In the absence of SOC ($\alpha = 0$), we can easily derive the number of edge states by algebraic arguments applied to equation (5). For $\epsilon_A = V, \epsilon_B = -V$ the equations become

$$\begin{align*}
(E - V) \Psi_{\mu_{A,i}} &= t \sum_j \Psi_{\mu_{B,j}}^\dagger \\
(E + V) \Psi_{\mu_{B,i}} &= t \sum_j \Psi_{\mu_{A,j}}^\dagger 
\end{align*}$$  \hspace{1cm} (6a)

$$\begin{align*}
(E - V) \Psi_{\mu_{A,i}} &= t \sum_j \Psi_{\mu_{B,j}}^\dagger \\
(E + V) \Psi_{\mu_{B,i}} &= t \sum_j \Psi_{\mu_{A,j}}^\dagger 
\end{align*}$$  \hspace{1cm} (6b)

We observe that for $E = -V$, equation (6b) transforms to the homogeneous set of $N_B$ equations with $N_A$ unknowns $0 = t \sum_j \Psi_{\mu_{B,j}}^\dagger$, which can only be satisfied by assuming that the amplitude on A sites is zero ($\Psi_{\mu_{A}}^\dagger = 0$) since $N_B > N_A$, i.e. the system is overdetermined with more equations than unknowns. On the other hand, equation (6a) transforms to $-2V \Psi_{\mu_{A}}^\dagger = t \sum_j \Psi_{\mu_{B,j}}^\dagger \Rightarrow 0 = t \sum_j \Psi_{\mu_{B,j}}^\dagger$, which is a homogeneous set of $N_A$ equations with $N_B$ unknowns, giving amplitudes $\Psi_{\mu_{B}}^\dagger$. This set of equations is an underdetermined system, since it contains fewer equations than unknowns, and therefore accepts $N_B - N_A$ linearly independent solutions.

Consequently for $\alpha = 0$ there are $N_B - N_A$ states at $V = 0$ with non-zero amplitudes only on the B sublattice sites. For $V = 0$ we derive the well-known case of bipartite lattices where there are at least $N_B - N_A$ states at $E = 0$ [53]. With the
application of the staggered potential ($V \neq 0$) the energy of these states is shifted to $E = -V$. Counting the spin degree of freedom also, these states become doubly degenerate.

The states at either $E = 0$ or $E = -V$ are edge states, with their corresponding wavefunctions concentrated at the zig-zag edges of the flake. The edge-state mechanism can be robustly understood by isolating part of the zig-zag edge as shown in figure 1 to the left of the flake schematic, where there are three B sites surrounding one A site. The underlying mechanism of the edge states can be visualized or schematically represented as two incoming electronic waves from the B sites 1 and 2, interfering and giving an outgoing wave at site 3 via the central A site. A phase difference between the wavefunction amplitudes on the respective sites 1 and 2 is introduced by Bloch’s theorem, as can be proved easily in a semi-infinite graphene sheet with one zig-zag edge [28]. For $E = 0$, interference between the waves from sites 1 and 2 results in zero amplitude at site 3 for states at the ends of the Brillouin zone where the phase difference is $\pi$ (destructive interference) or in a reduced amplitude otherwise. The interference mechanism continues inside the rest of the honeycomb lattice, being present whenever zig-zag edges exist at the borders of a confined graphene structure. The application of the staggered potential does not alter the basic topology of the honeycomb lattice that is responsible for the edge states, since it gives a potential $-V$ on all the B sites 1, 2, 3 and potential $V$ on site A, resulting in the shifting of the edge-state mechanism to energy $E = -V$. We note that the interference mechanism responsible for the edge states vanishes for the armchair edge morphology.

According to the above algebraic arguments, the energy of the edge states can be shifted to the opposite (conduction) side of the energy spectrum at $E = V$ by simply exchanging the potential on A and B sublattice sites, so that the outermost sites at the zig-zag edges in figure 1 have on-site potential $V$ instead of $-V$. In this way, the energy of the edge states can be tuned at either the valence or the conduction band edge by exchanging A- and B-type atoms, which can be achieved by cutting the trigonal flake in different orientations. We summarize that for Dirac flakes with zig-zag edges, in the absence of SOC, there are at least $|N_A - N_B|$ edge states at $E = V$ ($E = -V$) when the potential of the outermost atoms of the zig-zag edges is $V$ ($-V$). Therefore, there are always edge states whose energy is determined by the type of atoms at the zig-zag edges of the flake, while their number increases linearly with the system size $L$ as $|N_A - N_B| = L - 1$. 

![Figure 2](image-url)
We have verified our analytical results numerically. An example can be seen in figure 2(a) where the energy levels for a trigonal flake with $L = 8$ ($N_A = 45, N_B = 52$) and $V = 0.4$ are shown, near the energy gap. All states come in pairs due to the spin degeneracy, which is preserved even for finite $\alpha$. In agreement with our algebraic arguments there are $2(N_B - N_A) = 14$ edge states at $E = -V$ for $\alpha = 0$. When the SOC is introduced into the system, for $\alpha = 0$, the edge states disperse gradually inside the gap that is created, either due to the staggered potential $V$ or due to the finite flake size. This behavior can be attributed to the SOC term in equation (5), which alters the values of $E$ for which these equations can be satisfied. For sufficiently large $\alpha$ the states tend to repel, becoming almost homogeneously distributed inside the whole gap, despite being initially concentrated at its lower end ($E = -V$) for vanishing or small $\alpha$. A qualitatively similar behavior for the energy levels has been observed in MoS$_2$ flakes [25].

In general a significant interplay between the SOC and the staggered potential $V$ is expected, since both open a bulk gap at the Fermi energy. Additionally, the edge states due to zig-zag edges become gradually mixed with the edge states created by the SOC in analogy with the edge-state mechanism in the quantum Hall effect. In this sense, the edge-state mechanism originating from the honeycomb lattice structure is enhanced by the SOC, but its contribution is minimized for strong SOC.

In the simulation of certain materials the SOC term of equation (3) has to be applied on only one of the sublattices [46]. If it is applied only on A then the results we derived for $\alpha = 0$ remain valid, since the wavefunction amplitude on A sites is zero and any perturbation applied on this sublattice will not affect the edge states.

Some examples of these edge states can be seen in figures 2(b)–(d) where the wavefunction probability amplitude is shown, represented by the radius of circles at each site. The wavefunctions are obtained by the eigenstates of the diagonalized Hamiltonian blocks for each spin state in the Kramers doublet, up and down, which are decoupled. Since the wavefunctions are identical for the two states, only the wavefunction for one of the spin states is shown. For $\alpha = 0$ the amplitude of the edge state at $E = -0.4$ is non-zero only on the B sites, with the largest amplitude residing along the edges. The wavefunction becomes even more concentrated at the zig-zag edges for finite $\alpha$ with a slight diffusion in the bulk. A gradual accumulation at the corners of the triangle can be observed for strong SOC ($\alpha = 0.5$). This can be attributed to the different lattice connectivity between the sites at the corners of the triangle and those along the zig-zag edge. In particular, the corner sites are connected via two spin-dependent hoppings to second-nearest neighbors, instead of via four for sites along the zig-zag edge, as a consequence of equation (3). Also, each of the corners can be thought of as the intersection between two zig-zag chains causing additional interference effects, which cannot be distinguished for $\alpha = 0$ since the wavefunction probability is zero on the corner A sites, due to the bipartite nature of the honeycomb lattice. The wavefunction amplitude becomes gradually finite on all the A sites as $\alpha$ is increased, although it maintains different weights between the two sublattices.

4. Transmission probabilities

In the current section we investigate the transmission probabilities via the edges of the trigonal Dirac flakes with SOC. In order to probe the transmission we form a three-terminal device setup by attaching linear chains at the three corners of the triangle on A sublattice sites, as shown in figure 1. In figure 3 we show the spin-dependent transmission probabilities $T_{21}^{\alpha}$ for $L = 8$ along one side of the triangle between leads 1 and 2 for the spin-up and spin-down cases. We have performed the calculation for different values of the staggered potential $V$ and the SOC strength $\alpha$. The electronic flow
inside the energy area where we plot our results is carried via edge states like those in figure 2 for finite $\alpha$. For weak SOC ($\alpha = 0.05$) resonant transmission near the respective energy levels of the system can be seen as sharp peaks. Increasing $\alpha$ causes broadening of these peaks, resulting in the smooth fluctuations shown. A significant difference between the opposite spins is starting to appear for sufficiently large $\alpha$. For $\alpha = 0.5$ a small regime is formed for every $V$, indicated with a small arrow, where there is almost perfect propagation of solely spin-up electrons ($T_{21}^\uparrow \approx 1$, $T_{21}^\downarrow \approx 0$).

The spin-polarized regime is shifted slightly with increasing $V$. This can be attributed to the scattering via the positive potential $V$ from the leads that is encountered by the incident electrons, which can be thought of as a barrier that the electrons need to overcome by acquiring sufficiently large incident energy $E$. We have verified numerically that the transmission probabilities $T_{ij}^\mu$ between different leads satisfy the conditions $T_{ij}^\mu = T_{ji}^\mu$, which along with the symmetry of the triangle ensure that

$$
T_{21}^\uparrow = T_{32}^\uparrow = T_{13}^\uparrow = T_{23}^\uparrow = T_{12}^\uparrow = T_{31}^\uparrow = T_{21}^\downarrow = T_{32}^\downarrow = T_{13}^\downarrow = T_{23}^\downarrow = T_{12}^\downarrow = T_{31}^\downarrow = 1,
$$

$$
T_{21}^\uparrow = T_{21}^\downarrow = T_{32}^\uparrow = T_{32}^\downarrow = T_{13}^\downarrow = T_{13}^\uparrow = T_{12}^\uparrow = T_{12}^\downarrow = T_{31}^\uparrow = T_{31}^\downarrow = 0,
$$

as shown on the right-hand side of figure 1. Therefore electrons propagating in opposite directions along the border of the flake will also have opposite spins, i.e. they become helically spin-polarized for sufficiently strong SOC. The helical behavior is essentially a consequence of the mechanism that also produces helical edge states in zig-zag nanoribbons with SOC [37]. In this section, our system can be considered as a flake version of a QSH system, the two being topologically equivalent. An additional mechanism that could affect the helicity is revealed by a careful observation of the zig-zag edge. In figure 1 we can see that the electronic flow along each side of the triangle will be split into two parts, one via the outermost B (black) sites and one via the innermost A (red) sites, which are carried via opposite turns corresponding to opposite spin-dependent amplitudes $\psi_1$ in equation (3). The flow via the A sites is partially suppressed since the wavefunction amplitude is generally smaller than on B sites, being a remnant of the bipartite nature of the system for $\alpha = 0$, which results in different weights between the two sublattices, as we have shown in the previous section. However, the contribution of this mechanism is minimized for strong SOC as the two weights balance gradually.

We observe that the transmission is higher for large $\alpha$ due to the accumulation of the wavefunction at the corners of the triangle where the leads are attached (A sites), as can be seen in figure 2(d). On the other hand, for small $\alpha$ the transmission is generally lower, since the wavefunction amplitude on those sites is small, making it harder to detect the helicity. Altering the position of the leads near the corners of the triangle can quantitatively affect our results due to a slight diffusion of the edge states in the bulk of the flake; however, the system becomes less sensitive for large $\alpha$, which minimizes the bulk diffusion. We have observed that, for weak SOC, it is possible to increase the degree of helical polarization $T_{21}^\uparrow$ detected at the leads, by appropriately placing them in different positions near the corners of the flake. Altering the position of the leads could provide a way of tuning the helical behavior in an experiment.

To further analyze the helical regime, in figure 4(a) we show a density color plot of the spin transmission $T_{21}^\uparrow$ versus $E$ and $\alpha$, along with individual cases for constant $\alpha$ in figure 4(b). The helical (yellow) regime can be clearly distinguished where $T_{21}^\uparrow$ becomes maximum ($T_{21}^\uparrow = 1$), signifying helically spin-polarized electrons that propagate along the flake’s border. We notice that for larger $V$, corresponding to materials with wider gaps, larger SOC is needed in order to observe the helically polarized electrons. This is due to the non-trivial interplay between the staggered potential $V$ and the SOC, which both open a bulk gap at the Fermi energy. The SOC has to be sufficiently strong that helical edge states can appear inside the gap generated by $V$, i.e. the SOC has to dominate the gap over $V$ [37, 54, 55]. The helical regime is retained for all flake sizes, ranging from tens to a few hundred atoms, as can be seen in figure 5, with more fluctuations created, due to the denser energy levels for larger flake sizes.

By appropriately tuning the chemical potentials $\mu_i$ of the reservoirs at the ends of each lead $i$ in the three-terminal setup, spin-polarized currents with different polarizations flow in each lead. By using equation (7), i.e. by assuming that spin up (down) rotates clockwise (antclockwise), the following matrix equation for a three-terminal setup, relating the spin currents $I_i^\uparrow$ in different leads with their respective chemical potentials, can be derived [55]:

$$
\begin{pmatrix}
I_1^\uparrow \\
I_2^\uparrow \\
I_3^\uparrow
\end{pmatrix} = \frac{e}{4\pi} \begin{pmatrix}
0 & 1 & 1 \\
1 & 0 & -1 \\
-1 & 1 & 0
\end{pmatrix}\begin{pmatrix}
\mu_1 \\
\mu_2 \\
\mu_3
\end{pmatrix}.
$$

For instance, for $\mu_1 = \mu_3$, opposite spin currents $I_1^\uparrow = -I_3^\uparrow = \frac{e}{4\pi}(\mu_1 - \mu_2)$ flow in leads 1 and 3. The respective charge currents do not vanish in this case, in conjunction with the QSH effect, and therefore the currents flowing in leads 1 and 3 are not pure spin currents but spin-polarized currents instead. Consequently, spin-resolved transport via different sides of the flake is possible, allowing in this sense a geometrical manipulation of the electron spin, since the paths of the spin-polarized electrons can be controlled by the flake’s shape. This could also be considered as a geometrical spin-splitting via the geometry of the flake.

We expect similar phenomena for flakes of a different shape, such as hexagonal, which could offer additional possibilities to control the spin-dependent transmission by attaching more leads at the flake’s corners. Also impurities or weak disorder should not affect our results since the system is protected from backscattering, as in QSH systems.

In order to further investigate the helical mechanism we introduce a simple model consisting of a triangle with just three sites with constant on-site potential $V$ in analogy to the potential at the corners of the flake in figure 1 and three linear chains attached to its corners acting as leads, as shown in figure 6(a). In order to simulate the effect of the SOC, we
I Kleftogiannis and I Amanatidis consider spin-dependent hoppings of strength $\alpha$ inside the triangle (see appendix A). This model can be considered as an isolation of the SOC mechanism for each sublattice A or B (equation (3)) inside one single hexagon in the honeycomb lattice, corresponding to $L=1$ for the trigonal Dirac flake. Alternatively it can be thought of as a robust simulation of the numerical model, since it contains the basic ingredients of the problem, namely the fact that the electrons propagate in an almost straight path along the border of the trigonal flake via the edge states, under the influence of the intrinsic SOC. We note that, due to the way we oriented the triangle, the spin transmission from site 1 to 2, $T_{21}^s$, takes negative values, and therefore in figure 6(b) we show $-T_{21}^s$ in order for it to lie on the positive axis, for different $V$ and SOC strengths. The

Figure 4. (a) Density color plot of the spin transmission versus $E$ and $\alpha$. In the yellow area where $T_{21}^s \approx 1$ the electrons are helically spin-polarized. Larger $\alpha$ is required for materials with wider gaps (larger $V$) in order to observe the helicity. (b) Some corresponding cases of $T_{21}^s$ versus $E$ for different $\alpha$.

Figure 5. $T_{21}^s$ for $\alpha = 0.5$ and different flake sizes $L$. The helical regime is retained for all $L$ independently of $V$. 
details of the calculation are presented in the appendix A. The analytical curves catch the trend of the numerical results for the trigonal flake with maximum $T_{21} \approx 1$ for sufficiently large $\alpha$, which is shifted in energy for finite $V$.

5. Concluding remarks

We have presented a numerical study of the spin properties of electrons in flakes made of Dirac materials in the presence of intrinsic spin–orbit coupling (SOC). A detailed analysis of the edge states is also presented, based on sublattice arguments. The flakes are simulated by an effective tight-binding model involving a honeycomb lattice with staggered sublattice potential, which can be thought of as a numerical version of the Dirac equation. We probe the spin-dependent transport by forming a multi-terminal device that allows the calculation of the transmission probabilities along the edges of the flakes via the Green’s function formalism.

We have found that for vanishing or weak SOC the edge states are concentrated at either the valence or the conduction edge of the energy spectrum, depending on the on-site energy of each sublattice, with different wavefunction weights between the two sublattices. The edge states disperse gradually inside the gap as the SOC strength is increased. The electrons propagating along the border of the flakes via the edge states become helically spin-polarized for strong SOC, for both the massless and massive cases, corresponding to Dirac materials with and without a gap at the Fermi energy, respectively. The helicity can be easily detected in a three-terminal setup formed naturally by attaching 1D leads at the corners of a trigonal flake. Appropriate tuning of the chemical potential of each lead creates spin-resolved electronic transport via the different sides of the flake, allowing a geometrical manipulation of the electron spin.

In other words, we have shown that spin-resolved transport can be created intrinsically in flakes made of Dirac materials by forming multi-terminal devices without the need for external fields, the only requirement being sufficiently strong intrinsic SOC. We hope that our work will motivate further investigation of the SOC effects in 2D materials in conjunction with topological effects due to confinement in flakes and other nanostructures.

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Appendix A. Simple model

In the following appendix A, we present the derivation of the transmission probabilities for a simple system consisting of a triangle with three sites, and three linear chains attached to its corners acting as leads. We consider SOC inside the triangle by assuming spin-dependent hopping of strength $\alpha$ between sites, in analogy with the numerical model. Spin up (down) corresponds to $\mu = 1 (-1)$.

The Hamiltonian of the system can be split into spin-up and spin-down blocks, since the SOC does not mix the two spins, as

$$H = \begin{pmatrix} h^u & 0 \\ 0 & h^d \end{pmatrix} \quad (A.1)$$

where $h^u$ and $h^d$ are

$$h^u = \begin{pmatrix} V & 1 - i\mu \alpha & 1 + i\mu \alpha \\ 1 + i\mu \alpha & V & 1 - i\mu \alpha \\ 1 - i\mu \alpha & 1 + i\mu \alpha & V \end{pmatrix} \quad (A.2)$$

Figure 6. (a) A simple model simulating the three-terminal setup of the trigonal Dirac flake, the edge-state mechanism and the influence of the intrinsic SOC. (b) $T_{21}$ for different $\alpha$ and $V$. The curves describe the trend of the numerical results for all cases.
by assuming real hopping $t = 1$ eV between the three sites, with $\mu = 1$ ($-1$) for spin up (down). The transmission probabilities between the different sites of the triangle can be calculated via the Green’s function

$$G(E) = (E I - H - \Sigma(E))^{-1}$$  \hspace{1cm} \text{(A.3)}

where $\Sigma(E) = \Sigma_1(E) + \Sigma_2(E) + \Sigma_3(E)$ is the self-energy due to the semi-infinite linear chains at the corners, described by $H_{1D} = \sum_{\alpha \beta} (c^+_{\alpha \beta} c_{\alpha \beta} + c^+_{\alpha \beta} c_{\alpha \beta})$ with energy dispersion $E = 2 \cos(k)$. $\Sigma(E)$ is given by equal diagonal blocks for spin up and down:

$$\Sigma_{\mu}(E) = \begin{pmatrix} \Sigma_{1D}(E) & 0 & 0 \\ 0 & \Sigma_{1D}(E) & 0 \\ 0 & 0 & \Sigma_{1D}(E) \end{pmatrix}$$  \hspace{1cm} \text{(A.4)}

where $\Sigma_{1D}(E)$ is the self-energy of each chain, which can be calculated as follows [56].

Consider the surface Green’s function of the chain $g(E)$. Adding a single site via hopping $s$ at the point of excitation, giving the self-energy $\Sigma_{1D}(E)$, where

$$g(E) = (E - g(E))^{-1} \Rightarrow g(E) = \frac{E}{2} \pm \frac{E^2}{4} - 1.$$  \hspace{1cm} \text{(A.6)}

Since we are interested only in the retarded Green’s function we choose the minus sign representing outgoing waves from the point of excitation, giving the self-energy $\Sigma_{1D}(E) = g(E)$,

$$\Sigma_{1D}(E) = \frac{E}{2} - i \sqrt{1 - \frac{E^2}{4}} \text{ for } -2 < E < 2.$$  \hspace{1cm} \text{(A.7)}

Since $H$ and $\Sigma(E)$ are both block-diagonal in the spin basis, this is also true for equation (A.3). Therefore the Green’s function elements between opposite spins are zero, and we can write

$$G^\mu(E) = (EI - h^\mu - \Sigma^\mu(E))^{-1}. \hspace{1cm} \text{(A.8)}$$

By plugging equations (A.2) and (A.4) into equation (A.8) and inverting, we derive the following formula for the Green’s function element from site 1 (excitation) to site 2 (response):

$$G_{12}^\alpha(E) = \frac{1 - \alpha^2 + E - \Sigma_{1D}(E) + i \mu (2 - E - \Sigma_{1D}(E) - V) - V}{(2 - E + \Sigma_{1D}(E) + V)(-3\alpha^2 + (1 - E + \Sigma_{1D}(E) + V)^2)}.$$  \hspace{1cm} \text{(A.9)}

In order to calculate the respective transmission probabilities we apply the Fischer–Lee relations [51],

$$T_{12}^\alpha(E) = \nu(E)^2 |G_{12}^\alpha(E)|^2$$  \hspace{1cm} \text{(A.10)}

where $\nu(E) = \frac{\partial E}{\partial k} = -2\sqrt{1 - \frac{E^2}{4}}$ is the group velocity of the linear chains, assuming that $\hbar = 1$. We note that the transmission probabilities between opposite spins are zero since the respective Green’s function elements are zero.

By using the above relation we can calculate the spin transmission $T_{12}^s(E)$, which is plotted in figure 6:

$$T_{12}^s(E) = T_{12}^U(E) - T_{12}^D(E).$$  \hspace{1cm} \text{(A.11)}

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