Orbital magnetic moments induced by spin-orbit coupling in Dirac systems: Impact on magnetotransport in graphene van der Waals heterostructures

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In honeycomb Dirac systems with broken inversion symmetry, orbital magnetic moments coupled to the valley degree of freedom arise due to the topology of the band structure, leading to valley selective optical dichroism. In this paper we show that orbital magnetic moments emerge in the presence of spin-orbit coupling in such systems as well. We find that these moments are coupled to spin, but otherwise have the same functional form as the moments stemming from spatial inversion breaking. In other words, the moments are opposite for opposite spins, leading to g-factor renormalization. Such a duality is found to reflect on the Landau level spectrum, particularly on the zeroth Landau level. While these findings are relevant for a whole set of newly discovered materials, such as silicene and germanene, we subsequently focus on the particular impact that these moments have on graphene barriers with artificially engineered spin-orbit coupling. We study transmission properties of such barriers in the presence of a magnetic field. The orbital moments are found to manifest in transport characteristics through spin-dependent transmission and conductance, making them directly accessible in experiments. We find that a quasiclassical view thoroughly explains all the observed phenomena.

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I. INTRODUCTION

One of the more intriguing recent developments in the field of graphene research is artificial generation of properties otherwise vanishing in intrinsic samples. For instance, carrier mass can be created by sandwiching graphene with hexagonal boron nitride (hBN), in which case a gap arises for sufficiently aligned layers.1,2 The occurrence of the gap is dictated by the interplay of the elastic energy of the graphene lattice, and the potential energy landscape stemming from hBN.1 The energetically preferred commensurate structure, in which a carbon atom sits over a nitrogen atom, will maximize its area at the expense of other stacking configurations by stretching of the graphene layer. This in turn leads to the appearance of an average gap in the resulting van der Waals heterostructure.2

On the other hand, it was postulated that spin-orbit coupling (SOC) in graphene can be enhanced by hydrogen adsorption, which forces local rehybridization of bonds.3 Note that quantum spin Hall transport signatures introduced by random adatoms are well described by models taking into account a renormalized and uniform SOC. Moreover, proximity effect caused by an appropriate substrate was speculated to lead to SOC enhancement as well. Both of these mechanisms were recently confirmed experimentally, opening new venues for theoretical research.4,5

While in graphene carrier mass and SOC have to be artificially engineered, they are ubiquitous in other group IV monolayers such as silicene, germanene and stanene, thanks to a buckled structure and heavier constituent atoms.6,7,8 Given their honeycomb lattice, they also belong to the same class of materials with relativistic quasiparticles described by the Dirac equation, as does graphene. From this theoretical point of view, both aforementioned parameters appear in a similar form in the low energy continuum picture. They are captured by staggered potential terms Δ and Δ_SO in the case of mass and SOC, respectively. The term staggered potential originates in the language of the tight binding method, and refers to the breaking of the sublattice symmetry by a traceless potential. Unlike SOC, for which the staggered potential changes sign depending on the spin and valley of the electron, Δ opens up a topologically trivial band gap in the vicinity of the K and K′ points through the inversion symmetry breaking.

At the same time however, the inversion symmetry breaking leads to a nontrivial alteration of the semiclassical equations of motion on a honeycomb lattice.12,13 The quantum corrections, which reflect the impact of the Berry phase, and are therefore topological in nature, are twofold. On one hand, when subjected to an electric field in the plane, massive Dirac fermions will attain a velocity component transverse to the field, which is opposite in opposite valleys, thus giving rise to the valley Hall effect. This effect was recently observed experimentally in a MoS2 device.14 On the other hand, self-rotation of the wavepackets near the two valleys will produce valley-contrasting orbital magnetism.15

It is well established that the valley Hall and intrinsic spin Hall effects share the same origin, reflecting the Berry curvature properties of the underlying system. Therefore, the two Hall effects are fully analogous.15,16 Whereas the case of the valley-contrasting magnetism has been explored in Ref. 15, the analysis of the corresponding spin analogue in honeycomb crystals has not been previously explored. Recently we found evidence...
II. ORBITAL MOMENTS IN THE TIGHT BINDING PICTURE

We start with the low-energy tight binding Hamiltonian valid for a whole set of Dirac materials with prominent intrinsic spin-orbit coupling,

$$H = \hbar v_F [\tau k_x \sigma_x + k_y \sigma_y] + s \tau \Delta_{SO} \sigma_z, \quad (1)$$

where $v_F$ is the Fermi velocity, $\Delta_{SO}$ is spin-orbit coupling, $\sigma_i$ is a Pauli matrix operating in the sublattice subspace, $s = +1/-1$ labels the spin $\uparrow/\downarrow$, and $\tau = +1/-1$ labels the valley $K/K'$. As already mentioned this form of SOC is universal to all group IV monolayers other than graphene, in which it could be artificially generated as already mentioned. Note that here $k_x$ and $k_y$ are only parameters, and not operators. The dispersion relations extracted from Eq. (1) are shown by thin lines in Fig. 1(a).

The Hamiltonian (1) describes a two-state, electron-hole symmetric system. For such systems, the orbital magnetic moment ($m$) is directly proportional to the Berry curvature ($\Omega$), $m \sim \Omega$ [13,15]. On the other hand, the system is also time-reversal invariant, and since we disregard the staggered potential $\Delta$ at the moment, inversion symmetry is not broken either. Since for spatial-inversion and time-reversal symmetric systems Berry curvature vanishes [19,20], one might conclude that the orbital moments must vanish as well. However, it is rarely stressed that this only holds for spinless electrons, which is not the case considered here [21]. In fact, the Hamiltonian (1) describes a topological insulator, having a non-zero and opposite Chern numbers for opposite spins. This is because spin-orbit coupling mimics spin-dependent magnetic field, thus breaking the time-reversal symmetry separately in each spin sector. Since the Chern number is obtained as an integral of $\Omega$ over the Brillouin zone, the Berry curvature is therefore nontrivial; consequently, orbital magnetic moments will be nonzero as well.

The orbital moments originate from the self-rotation of the electron wave packet around its center of mass, and can be obtained from the tight binding Bloch eigenfunctions $|u(k)\rangle$ [19]

$$m = -i \frac{e}{2\hbar} [\nabla_k u] \times [H - E(k)] |\nabla_k u\rangle, \quad (2)$$

which makes their topological origin much clearer. For the particular Hamiltonian in Eq. (1), we have

$$|u(k)\rangle = \left( \tau \alpha \sqrt{ \frac{E + \Delta_{SO}}{2E} } e^{i\phi} \right), \quad (3)$$

where $E$ is the electron energy, $\alpha = +1$ ($\alpha = -1$) denotes the conduction (valence) band, and $\phi = \arctan k_y/k_x$. It is then straightforward to show that the expression for the magnetic moments which arise from the spin-orbit coupling reads

$$m = -s \frac{e \hbar v_F^2 \Delta_{SO}}{2(\Delta_{SO}^2 + \hbar^2 v_F^2 k^2)}, \quad (4)$$

Variations of the orbital moments in the vicinity of the Dirac points are shown for both spins in Fig. 1(a). They

![FIG. 1. The orbital magnetic moments of the spin-up (spin-down) states shown by thick red (dashed blue) lines, and the corresponding low-energy band structure, shown in black, for: (a) $\Delta = 0$ and $\Delta_{SO} = 30$ meV, and (b) $\Delta = 30$ meV and $\Delta_{SO} = 0$. Note that in (b) the orbital magnetic moments for the two spins are equal, due to the absence of SOC.](image-url)
are maximum near the band edges, decay away from the two Dirac points, and are obviously opposite for opposite spins.

One can compare these moments with the valley-contrasting moments, arising for $\Delta_{SO} = 0$ and $\Delta \neq 0$. Their magnitude is given by

$$m = -\tau \frac{\hbar v_F^2 \Delta}{2(\Delta^2 + \hbar^2 v_F^2 k^2)},$$

and they are depicted in Fig. 1b. It becomes clear that the two sets of moments share a similar functional form, except the former couple to spin, while the latter couple to the valley degree of freedom.

In the case of nonzero both $\Delta_{SO}$ and $\Delta$, and in the low energy limit, the magnetic moment is given by

$$m = -\frac{\hbar v_F^2}{2(s\Delta_{SO} + \tau \Delta)}.$$  

Note that one could have also arrived at the above expression by simply replacing $\Delta$ with $s\tau\Delta_{SO} + \Delta$ in the low energy limit derived in Ref. 13.

The orbital magnetic moments are responsible for the optical selection rules of light absorption in Dirac materials, through the so-called circular dichroism effect. Note that the orbital moments in Eq. 1 can dominate the Zeeman response of a system, since they can be orders of magnitude stronger than the free electron Bohr magneton for realistic SOC strengths found in typical Dirac materials. In other words, they will lead to renormalization of the Landé $g$ factor, which was recently observed for transition metal dichalcogenides from first-principle calculations presented in Ref. 23.

### III. LANDAU LEVELS, PSEUDOSPIN POLARIZATION AND ORBITAL MOMENTS IN THE CONTINUUM PICTURE

We proceed with the case of an applied perpendicular magnetic field $\mathbf{B} = B\hat{e}_z$, for which we employ the Dirac-Weyl Hamiltonian

$$H = \hbar v_F \left[ \tau k_x \sigma_x + (k_y + \frac{e}{\hbar} A_y) \sigma_y \right] + s\tau\Delta_{SO} \sigma_z + \Delta \sigma_z.$$  

This equation could be employed to solve the electron spectrum in the Dirac systems in the presence of $\Delta_{SO}$, $\Delta$, and magnetic field. It will subsequently lead us to resolve the magnetic moments. Here, the Landau gauge $A = (0, A_y)$, $A_y = Bx$ is chosen. In this gauge $k_y$ is a good quantum number and the solutions have the form $\Psi(x, y) = \exp(ik_y y)(\psi_A(x), \psi_B(x))^T$. Introducing $\hbar v_F E = E$, $\hbar v_F \delta = \tau s\Delta_{SO} + \Delta$, one can find out the LLs in the infinite graphene sheet. In solving the LL spectrum it is useful to adopt the operators $b^\dagger_\tau = -i(\hbar B/\sqrt{2}) (\tau k_x + ik_y + i e A_y/\hbar)$ and $b_\tau$, where $l_B = \sqrt{\hbar/eB}$ denotes the magnetic length. $b_\tau^\dagger$ and $b_\tau$ are the bosonic ladder operators, since they satisfy $[b_\tau, b_\tau^\dagger] = \tau$. It could be useful to define these operators such that they fully correspond to the standard ladder operators of the quantum harmonic oscillator (QHO) shifted by $x_0 = k_F^2 l_B^2$ and having the mass $m = \hbar^2/l_B^4 k^2$.

Then the eigenstates will be given by the standard (obviously shifted and rescaled) QHO solutions

$$\langle x|n \rangle = \frac{1}{\sqrt{2^n n!}} e^{-(x/l_B + k_y l_B)^2/2} H_n \left( \frac{x}{l_B} + k_y l_B \right),$$

where $H_n$ are Hermite polynomials. The problem can now be solved in terms of these solutions for the case of the regular 2D electron gas in a magnetic field, having in mind that $b_\tau^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$, $b_\tau|n\rangle = \sqrt{n}|n-1\rangle$, and that the ladder operators change character in the $K'$ valley. The system of coupled equations with ladder operators is now given by

$$\delta \psi_A - \frac{i\omega_c}{v_F} b_\tau \psi_B = \epsilon \psi_A,$$

$$\frac{i\omega_c}{v_F} b^\dagger_\tau \psi_B - \delta \psi_B = \epsilon \psi_B,$$

where $\omega_c = \sqrt{2} v_F/l_B$ is the cyclotron frequency for Dirac-Weyl electrons. Then for $n \geq 1$ LLs themselves are given by

$$\epsilon_{n,s,\tau,\pm} = \pm \sqrt{\delta^2 + n \omega_c^2/v_F^2}.$$  

The $s$ and $\tau$ quantum numbers are contained implicitly in the definition of $\delta$. The joint spinor for the two valleys can be written as

$$|n, s, \tau, \pm\rangle = \left( \frac{|n - \tau - \frac{1}{2}\rangle}{\sqrt{(\tau + \tau)_{\pm}}} \right).$$

The case of $n = 0$ needs special attention, since the solution Eq. 12 is not valid. Then, the appropriate choice for the solution is

$$|0, s, \tau, \pm\rangle = (-\tau/2 + 1/2, \tau/2 + 1/2)^T |0\rangle,$$

while the level is expressed as

$$\epsilon_{0, s, \tau} = -\tau \delta.$$

Note that these eigenvectors and eigenvalues correspond exactly to the massless Dirac electron case, under the requirement $\delta \to 0$. In fact one could have arrived at the same LL spectrum by some simple argument, starting from the LL spectrum of massless graphene, $\epsilon_{n, \pm} = \pm \sqrt{n \omega_c^2/v_F^2}$, $n \geq 0$. Firstly for $n \geq 1$, the LL spectrum of gapless graphene is electron-hole symmetric, with electron and hole eigenstates related via the chiral symmetry $\psi_{n,-}^{\dagger} = \sigma_2 \psi_{n,+}^{\dagger}$. Moreover, their sublattice pseudospins lie in the horizontal plane, ensuring equal weight on both sublattices. Having this in mind, we can
than reintroduce $\delta$ and change the basis in a subspace made out of a particular electron-hole pair, resulting in

$$H'_n = \begin{pmatrix} \epsilon'_n & \delta \\ \delta & -\epsilon'_n \end{pmatrix}$$

(15)

whose diagonalization yields $\epsilon_{n,s,\tau,\pm} = \pm \sqrt{\delta^2 + \epsilon^2}$, as obtained by the ladder operators, Eq. [14]. On the other hand for $n = 0$, the spinor for the original massless LL spectrum is also given by Eq. [13], i.e. it is sublattice pseudospin polarized. Its sublattice pseudospin is pointing down in the $K$ valley, and up in the $K'$ valley, i.e. it equals $-\tau$. But now note that the SOC and the mass actually appear as a pseudo Zeeman term, acting on this sublattice pseudospin, Eq. [7]. Therefore this term will simply shift the original levels by $-\tau\delta$, which again returns Eq. [13] already obtained.

Thus the SOC and mass split and shift the zeroth LLs away from zero energy, and the sublattice pseudospin gets coupled with the valley pseudospin. This is similar to transition metal dichalcogenides,[23] with a difference here that for general $\Delta_{SO}, \Delta$ no spin degeneracy is found in either valley. In the $\delta = 0$ limit, the sublattice and valley pseudospin get coupled only at zero energy, whether or not the magnetic field is present.[24][25] Note that the duality $\Delta_{SO} \leftrightarrow \Delta, s \leftrightarrow \tau$ is present in Eq. [14]. In other words, SOC couples the LLs to spin in the same way that mass couples them to the valley degree of freedom.[23][24][25][26][27][28][29][30][31][32][33]

Note that the zeroth LLs always reside on the edges of the appropriate bands. Furthermore, upon interchanging $\Delta_{SO}$ and $\Delta$, there is switching of the $s\tau = -1$ zeroth LLs between the two bands. This can be seen from Eq. [14], since for $\Delta_{SO} \neq \Delta$ performing $\Delta_{SO} \leftrightarrow \Delta$ changes the sign of the $s\tau = -1$ LLs.

The underlying explanation for the behavior of the LL spectrum can be sought in the existence of orbital magnetic moments.[31][32] In a similar fashion to Ref. [22] we can obtain the effective Bohr’s magneton in the presence of $\Delta_{SO}$, starting from the Dirac-Weyl equation, and expanding near the conduction band bottom. We first point out that near the bottom of the conduction bands the sublattice pseudospins get polarized perpendicular to the graphene sheet, with majority of the weight concentrated on the A (B) sublattice for $\delta > 0$ ($\delta < 0$). Likewise, at the top of the valence band most of the weight is found on A (B) sublattice for $\delta < 0$ ($\delta > 0$). This is obvious for the zeroth LLs, but to see it for higher levels it is helpful to derive the expectation value for the sublattice pseudospin

$$\langle n, s, \tau, |s\tau| n, s, \tau, \pm \rangle = \frac{\delta}{\epsilon}$$

(16)

which is exactly the same as in the absence of SOC and magnetic field.[33] only now it is to be used for the discrete energy values corresponding to the Landau levels. Obviously having the form of a pseudo Zeeman term, $\delta$ is the main culprit for this polarization. Therefore, perfect pseudospin polarization is achieved in the bottom (top) of conduction (valence) band.

On the other hand, decoupling the Dirac-Weyl equation gives

$$\left[ k_z^2 + \left( k_y + \frac{x}{l_B} \right)^2 \pm \frac{\tau}{l_B^2} \right] \psi_{A/B} = (\epsilon^2 - \delta^2) \psi_{A/B}.$$ 

(17)

Therefore, there is a spatially uniform term proportional to the magnetic field, with opposite signs on opposite sublattices and opposite valleys. Consider the importance of this term for states whose sublattice pseudospin mostly lies in the graphene plane, i.e. for states far away from the band gap, Eq. [16]. For such states the two signs play a tug of war, effectively canceling each other out. However, near the band gap, sublattice polarization occurs, and the term corresponding to a majority sublattice starts dominating over the other, giving rise to an effective paramagnetic moment. For instance, when $\delta > 0$ sublattice A dominates for low electron energies, and the upper sign starts impacting the electron motion. To fully appreciate this fact, and write the equation in a manifestly paramagnetic form, one needs to do a low energy expansion for the equation of the majority sublattice. After reintroducing $E$, $\Delta$, and $\Delta_{SO}$ explicitly, we can write $E = \xi \pm (s\tau \Delta_{SO} + \Delta)$ for $\delta > 0$, and $E = \xi \mp (s\tau \Delta_{SO} + \Delta)$ for $\delta < 0$ in the conduction and the valence band, respectively. Taking the limit $\xi \rightarrow 0$, the following equation is obtained

$$\left[ \frac{\mu_{\text{eff}}^2}{2m_{\text{eff}}} + \left( \frac{e A_y}{2m_{\text{eff}}} \right)^2 \pm \frac{e \hbar v_F^2 B}{2(s\Delta_{SO} + \tau\Delta)} \right] \psi = \xi \psi.$$ 

(18)

where $m_{\text{eff}} = |s\tau \Delta_{SO} + \Delta| / v_F^2$ is the electron effective mass due to the band gap. This is the form of the Schrödinger equation in the presence of magnetic field in which the emerging magnetic moments are obviously manifested. Once again we see the duality of the orbital moments of the same nature as mentioned previously in the case of LLs: the moments are coupled to SOC through spin and to mass through valley degree of freedom. Moreover, it is obvious that the expression for the magnetic moment equals the results of low energy expansion in Eq. [16]. Having in mind that these moments effectively shift the low energy parabolic bands, one can use the same argument as in Ref. [31] to show that the separation between the lowest LL and the bottom of each shifted band is for each spin, valley and band equal to half the separation between this and the first excited LL to first order. This is in analogy with the LLs in a 2D massive-electron gas, where the lowest level sits at half the cyclotron frequency.[31][32] The difference in higher energy LLs follows due to the deviation of the dispersion from the quadratic one.
IV. TRANSMISSION THROUGH A BARRIER IN BULK GRAPHENE

We proceed with considering how the emerging moments affect transport properties. In particular, we analyze transport through a single 1D barrier in bulk graphene, in which the intrinsic SOC is modified. For the magnetic field to be included only in the barrier, we choose the following vector potential (within the Landau gauge)

$$A_y = \begin{cases} 
0 & x < 0 \\
Bx & 0 \leq x \leq W \\
BW & x > W 
\end{cases}$$

(19)

As mentioned, due to the translational invariance along the transpose direction $k_y$ is a good quantum number and the solutions have the form $\Psi(x, y) = \exp(ik_yy)(\psi_A(x), \psi_B(x))^T$. The following coupled system of differential equations is then obtained

$$\left(\tau k_x + ik_y + i\frac{\epsilon}{\hbar} A_y \right)\psi_{B/A} \pm \delta \psi_{A/B} = \epsilon \psi_{A/B}.$$  

(20)

Reducing the coupled system to a set of two independent second order differential equations leads to

$$\left[\partial^2_z + \tau^2 \left(\frac{\partial_x}{l_B^2} - (k_y + \frac{x}{l_B})^2 + \epsilon^2 - \delta^2\right)\right] \psi_{A/B} = 0.$$  

(21)

Having in mind the form of the vector potential, the differential equation in the barrier becomes

$$\left[\partial^2_z + \tau \left(\frac{\partial_x}{l_B^2} - (k_y + \frac{x}{l_B})^2 + \epsilon^2 - \delta^2\right)\right] \psi_{A/B} = 0,$$  

(22)

where $l_B = \sqrt{\hbar/\epsilon B}$ is the magnetic length. By using the transformation $z = \sqrt{2}(k_y l_B + x/l_B)$ the following equation is obtained

$$\left[\partial^2_z + 1/2 - 1/2 + \tau + (\epsilon^2 - \delta^2) \frac{l_B^2}{2} - \frac{z^2}{4}\right] \psi_{A/B} = 0.$$  

(23)

It has the form of the parabolic cylinder (Webers) differential equation

$$y'' + \left(\nu + \frac{1}{2} - \frac{z^2}{4}\right)y = 0,$$  

(24)

whose solutions are given in terms of parabolic cylinder functions

$$y = C_1 D_\nu(z) + C_2 D_{\nu+1}(z).$$  

(25)

Finally the solution for the first sublattice is given by

$$\psi_A = C_1 D_{\nu} \left[\sqrt{2}(k_y l_B + x/l_B)\right] + C_2 D_{\nu+1} \left[-\sqrt{2}(k_y l_B + x/l_B)\right],$$  

(26)

where $\nu_A = (\epsilon^2 - \delta^2) l_B^2/2 - \tau/2 - 1/2$. For the other sublattice after employing the recurrence relations

$$\frac{\partial D_\nu(z)}{\partial z} = \frac{1}{2} z D_\nu(z) - D_{\nu+1}(z),$$  

(27)

and the relationship (20), one gets the following expression

$$\psi_B = C_1 g D_{\nu_A} \left[\sqrt{2}(k_y l_B + x/l_B)\right] - C_2 g D_{\nu_A+1} \left[-\sqrt{2}(k_y l_B + x/l_B)\right],$$  

(28)

where $\nu_B = (\epsilon^2 - \delta^2) l_B^2/2 + \tau/2 - 1/2$, and

$$g = i \left[\sqrt{\frac{\tau}{2}} \right]^\tau \left(\epsilon + \tau \delta\right) l_B.$$  

(29)

If the relation

$$D_\nu(z) = 2^{-\nu/2} e^{-z^2/4} H_\nu\left(\frac{z}{\sqrt{2}}\right)$$  

(30)

is employed, the spinor multiplied by $C_1$ in Eqs. (26) and (28) reduces to the solution (12), once the incident energy is equal to a particular Landau level, as could be expected.

The incident wave function is given by

$$\psi_I = e^{ik_z x} \left(\frac{1}{\tau e^{\tau \phi}} \right) + re^{-ik_z x} \left(\tau e^{\tau \phi} \right),$$  

(31)

where $\phi = \arctan k_y/k_x$.

Finally, in the third region the vector potential is a non-zero constant, and employing the standard plane wave ansatz, the solution is given by

$$\psi_{III} = t \frac{k_x}{k_x} e^{ik_z x} \left(\frac{1}{\tau e^{\tau \phi}} \right),$$  

(32)

with the energy of the plane wave given by $\epsilon = \alpha \sqrt{k_x^2 + k_y^2}$, $k_x = \epsilon \cos \theta$, the effective transverse momentum after the barrier $k_y = \epsilon \sin \theta = k_y + W/l_B^2$ and $\theta$ being the angle of energy propagation. The additional factor under the square root follows from the current conservation. Again by replacing the expression for the momenta before and after the barrier, one can obtain the effective law of refraction for a barrier of thickness $W$ with nonzero $\Delta$, $\Delta_{SO}$ and $B$ as

$$\epsilon \sin \theta = \epsilon \sin \phi + W/l_B^2.$$  

(33)

The expressions for the wavefunctions in different regions, (31), (26), (28), and (32) are then matched at the interfaces $x = 0$ and $x = W$, which gives a system of equations, whose solution yields the transmission amplitude $t$

$$t = 2g\tau \cos(\tau \phi) \left(\sum_{\nu} G_{I\nu}^+ G_{I\nu} + \sum_{\nu} G_{III\nu}^+ G_{III\nu}\right) \frac{k_x}{k_x} \sqrt{k_x},$$  

(34)
\[ f = g^2 \left( F_A^+ G_B^- - F_B^+ G_A^- \right) + e^{i\beta(\theta-\phi)} \left( F_A^- G_A^+ - F_A^- G_A^+ \right) + g e^{i\phi} \left( F_B^+ G_A^+ + F_B^+ G_A^+ \right) + g e^{-i\phi} \left( F_A^+ G_B^+ + F_B^+ G_B^+ \right) . \]

(35)

Here the coefficients \( F^\pm \) and \( G^\pm \) are given by

\[ F_{A/B}^\pm = D_{\nu_{A/B}} \left[ \pm \sqrt{2} k y B \right] , \]

(36)

\[ G_{A/B}^\pm = D_{\nu_{A/B}} \left[ \pm \sqrt{2} (k y B + W / l_B) \right] . \]

(37)

V. RESULTS AND DISCUSSION

Since we analyze a barrier made exclusively out of SOC, the valley degree of freedom plays no role in electron transmission, which can be concluded from the theory presented in Sec. [II] and [III]. Therefore, the contour plots of the transmission coefficient \( T = |t|^2 \), for the two spin flavors, and for the 200 nm wide barrier as function of energy and incident angle of the incoming electron are shown in Fig. 2. Each horizontal panel in this figure corresponds to a specific value of the magnetic field, which is 0, 0.1, 0.2 to 0.3 T from top to bottom. Because of the duality \( \Delta_{SO} \leftrightarrow \Delta \) and \( s \leftrightarrow \tau \), the results presented below also apply for transmission through a barrier when \( \Delta \neq 0 \) and \( \Delta_{SO} = 0 \). But for this case the spin and valley quantum numbers should be interchanged.

For both barrier types, we found that magnetic field causes cyclotron motion, whose main feature is the appearance of a transmission window dependent on energy and angle \( \phi \). Outside of this window, the waves after the barrier become evanescent, and therefore no transmission takes place. This occurs when the longitudinal momentum \( k_x = \sqrt{\epsilon^2 - k_y^2} \) of each electron state in the region after the barrier becomes imaginary. The transmission window is given by

\[ \epsilon > \frac{\gamma}{1 - \sin \phi} , \]

(38)

where \( \gamma = W / l_B^2 \). The transmission windows for different \( B \) are shown by solid black lines in Fig. 2.

When magnetic field increases, the transmission asymmetry with respect to the incident angle becomes larger, due to the cyclotron motion, as Fig. 2 shows. Besides, whereas transmission coefficients are identical for both spins when no magnetic field is present, \( T_\uparrow \) and \( T_\downarrow \) differ when \( B \neq 0 \), which is a consequence of the SOC-induced magnetic moments. In fact, it is clear from Eq. (22) that a quasiclassical longitudinal momentum \( q_x \)

\[ q_x (x) = \sqrt{\epsilon^2 - \delta^2 - \left( k_y + x / l_B^2 \right)^2} - s / l_B^2 \]

(39)

can be assigned to the sublattice-polarized states.

![FIG. 2. Contour plots of the transmission coefficient as function of incident angle and energy for \( \Delta_{SO} = 30 \text{ meV}, \Delta = 0 \) and \( W = 200 \text{ nm} \). The magnetic field equals 0 T in (a-b), 0.1 T in (c-d), 0.2 T in (e-f), and 0.3 T in (g-h). The results are shown for both spin orientations. The semiclassical critical boundaries \( \epsilon_{cr} = 0 \) and \( \epsilon_{cr} = W \) are depicted by dash-dotted and dotted lines, respectively.](image)

In order to understand the effects of the emerging magnetic moments on transmission characteristics it is instructive to investigate how classical turning points vary with \( \epsilon \) and \( \phi \). Those turning points are extracted from \( q_x (x) = 0 \), where \( q_x \) is given by Eq. (39), and are given by

\[ x_{1,2} = -\epsilon l_B^2 \sin \phi + \frac{l_B^2}{\epsilon} \sqrt{\epsilon^2 - \delta^2 - \mu} , \]

(40)

where \( \mu = s / l_B^2 \) is the magnetic moment term which appears in the expression for the quasiclassical momentum in Eq. (39). Given that the barrier extends from 0 to \( W \), the condition that no turning points are found within the barrier is obtained by requiring \( x_1 < 0 \) and \( x_2 > W \). The former condition leads to

\[ x_1 < 0 \Rightarrow \begin{cases} \epsilon > \frac{\sqrt{\delta^2 + \mu}}{\cos \phi}, & \phi < 0 \\ \epsilon > \frac{\delta^2 + \mu}{\cos^2 \phi}, & \phi > 0 \end{cases} , \]

(41)

while the latter results in

\[ x_2 > W \Rightarrow \begin{cases} \epsilon > \frac{\sqrt{\delta^2 + \mu}}{\cos \phi} - \frac{\gamma}{\cos \phi}, & \epsilon \sin \phi + \gamma < 0 \\ \epsilon > \frac{\delta^2 + \mu}{\cos^2 \phi} + \frac{\gamma}{\cos \phi}, & \epsilon \sin \phi + \gamma > 0 \end{cases} . \]

(42)
On the other hand, both classically forbidden and classically allowed regions will be present in the barrier if $0 < x_1 < x_2 < W$. The two extreme cases of vanishing allowed regions occur when the leftmost turning point approaches the right interface of the barrier

$$x_1 < W \Rightarrow \begin{cases} \epsilon > \frac{\gamma \sin \phi + \sqrt{\gamma^2 + (\delta^2 + \mu) \cos^2 \phi}}{\cos^2 \phi}, & \epsilon \sin \phi + \gamma < 0 \\ \epsilon > \sqrt{\delta^2 + \mu}, & \epsilon \sin \phi + \gamma > 0 \end{cases}$$

and when the rightmost turning point approaches the left barrier interface

$$x_2 > 0 \Rightarrow \begin{cases} \epsilon > \sqrt{\delta^2 + \mu}, & \phi < 0 \\ \epsilon > \frac{\gamma \sin \phi + \sqrt{\gamma^2 + (\delta^2 + \mu) \cos^2 \phi}}{\cos^2 \phi}, & \phi > 0 \end{cases}$$

From the angle dependent functions in the last four equations one might define the critical energies

$$\epsilon_{cr0} = \frac{\sqrt{\delta^2 + \mu}}{\cos \phi},$$

and

$$\epsilon_{crW} = \frac{\gamma \sin \phi + \sqrt{\gamma^2 + (\delta^2 + \mu) \cos^2 \phi}}{\cos^2 \phi},$$

for which the classical turning points are located exactly at the two interfaces, i.e. they are obtained by solving $q_x (0) = 0$ and $q_x (W) = 0$, respectively. Those critical boundaries are plotted as dash-dotted and dotted lines in Fig. 2.

In order to elucidate the quasiclassical behavior, in Fig. 3(a) we plot the zones corresponding to different configurations of turning points by different colors. The same set of parameters is used as in Fig. 2(c) ($\Delta_{SO} = 30 \text{ meV}$, $W = 200 \text{ nm}$, $B = 0.2 \text{ T}$ and $s = +1$). In Fig. 3(b) we plot a set of classical trajectories which correspond to the zones shown in Fig. 3(a). As could be inferred from Fig. 2, for $\epsilon$ higher than both $\epsilon_{cr0}$ and $\epsilon_{crW}$ (green colored region in Fig. 3(a)), there is no classically forbidden region inside the barrier. However, if the electron energy is between the two critical energies (red or blue colored region in Fig. 3(a)), a classically forbidden energy range will appear on either end of the barrier. In other words the electron will have to tunnel through a part of the barrier adjacent to one of its interfaces, whereas propagation is free in the other part. For the most extreme case displayed as the magenta colored region in Fig. 3(a), the electron has to tunnel through both ends of the barrier.

One may notice that the two critical energies whose variation with $\phi$ is depicted by dash-dotted and dotted lines in Fig. 2 are almost identical for the two spins. Also, by careful inspection of Fig. 2 it becomes evident that quasiclassical zones we derived explain the observed transmission very well, especially for the spin up states. For the spin down states, however, transmission is enhanced with respect to the spin up states in the zones for which the electron waves must tunnel through a region of the barrier (the red and blue energy zones in Fig. 3(a)). This could be understood if one recalls that the WKB expression for the tunneling coefficient is given by

$$T \approx e^{-2Im \int q_\epsilon (x) dx}.$$  

where the integration is over a classically forbidden region. Having this in mind, it is obvious that for $\Delta_{SO} \neq 0$ and $B \neq 0$ spin-up states decay faster than the spin-down states in classically forbidden regions, due to the paramagnetic term. This difference increases at higher magnetic fields, which leads to increasing difference between the transmission coefficients for the two spins, as Fig. 2 clearly demonstrates. When the magnetic field is absent, the emerging paramagnetism vanishes, and therefore, the transmission characteristics for the two spins are identical (see Figs. 2(a) and (b)).

Next, we explore how presence of the magnetic moments affects the interference pattern shown in Fig. 2. This could be the most important effect from the practical point of view. In the Fabry-Perot model, the interference pattern depends on the phase the electron wave function accumulates between the barrier interfaces and the bounces from the interface(s) and/or turning point(s)

$$\alpha = \alpha_{WK} + \alpha_1 + \alpha_2,$$

where $\alpha_1$ and $\alpha_2$ are the backreflection phases, whereas
\[ \alpha_{WKB} \] is the WKB phase

\[ \alpha_{WKB} = 2 \int_{\max(0, x_1)}^{\min(W, x_2)} q_x(x) \, dx. \quad (49) \]

To analyze how the orbital magnetic moments influence the fringe pattern we could once again invoke Eq. (39) and the associated diagram in Fig. 2. It follows that Fabry-Perot resonances have different character in different zones. Whenever \( B \neq 0 \), the WKB phase is accumulated throughout the entire barrier for \( \epsilon > \max(\epsilon_{cr0}, \epsilon_{crW}) \), but only in region \([x_1, W]\) for \( \epsilon_{cr0} > \epsilon > \epsilon_{crW} \) (the red-shaded region in Fig. 2). Consequently, in the latter case the transmission maxima (depicted by red color in Fig. 2) are almost linear functions of \( \phi \), whereas in the former case their dependence on \( \phi \) is nonlinear.

The crucial point though, is that the phase accumulated during the propagation differs for different spin orientations. This occurs because magnetic moments associated with opposite spins contribute to \( \alpha_{WKB} \) in opposite ways (see eq. (39)). To see this clearly, and to provide experimentally verifiable predictions it is important to consider the conductivity of the entire studied structure, given as:

\[ G(\epsilon) = G_0 \int_{-\pi/2}^{\pi/2} T(\epsilon, \phi) \epsilon \cos \phi \, d\phi, \quad (50) \]

where \( G_0 = e^2 L / h^2 v_f \), with \( L \) denoting the lateral width of the entire structure in the \( y \) direction.

Since the effects of magnetic moments are most vividly manifested in dependence of \( dG/dE \) on energy, we display this quantity in Fig. 4 for the same set of parameters as in Fig. 2. Alongside with \( dG/dE \), the corresponding conductance is shown in insets for each case. As can be seen from these insets, \( G \) only depicts the fact that the spin-down conductance is increased with respect to the spin-up conductance, due to the enhanced transmission through the classically forbidden regions, as already discussed. On the other hand, the first derivative of the conductance with respect to energy conveys the information of the interference pattern, where the effects of the orbital moments are more transparent. Two issues are of importance here: (i) the difference between the two spins is clearly more pronounced at higher magnetic fields. This happens because in such a case the orbital moments have a larger impact on the electron dynamics, as pointed out before. (ii) The distinction between the two spins is more prominent at lower energies. This is a consequence of the larger emerging orbital magnetic moments of the electrons whose energies are close to the band edges than of more energetic electrons, as Eq. (41) and Fig. 1(a) demonstrate.

Finally, we would like to point out that the manifestations of orbital moments in transport properties can be captured by the tight-binding nonequilibrium Green function formalism as well. To show this, in Fig. 5(a) we plot a set of transmission curves obtained using the derived transmission amplitude (see Eq. (34)), while in Fig. 5(b) we plot the results of numerical transport simulations within the TB NEGF method, for the same barrier parameters. The model used to describe graphene in this case is given by
\[ H = -t \sum_{(i,j),\alpha} e^{i\varphi_{ij}} c^\dagger_{i\alpha} c_{j\alpha} + i\lambda_{SO} \sum_{(i,j),\alpha,\beta} \nu_{ij} e^{i\varphi_{ij}} c^\dagger_{i\alpha} s^z_{\alpha\beta} c_{j\beta}. \] (51)

The first term describes the usual hopping between nearest neighbor \( p_z \) orbitals in graphene, which extends beyond the barrier. The second term describes the intrinsic spin-orbit interaction found in the barrier, through the next-nearest-neighbor (NNN) hopping amplitude \( \lambda_{SO} (\Delta_{SO} = 3\sqrt{3}\lambda_{SO}) \). Note that \( \nu_{ij} \) determines the sign of the hopping: for spin up (down), hopping between counterclockwise coupled NNNs count as positive (negative), while hopping between clockwise coupled NNNs count as negative (positive). The Peierls term \( \varphi_{ij} = \frac{\xi}{\hbar} \int_{r_{ij}} A \cdot dl \) accounts for the phase the electron acquires while traveling in the presence of the magnetic field. The details of the NEGF procedure are given in Appendix A.

Although the continuum and the TB NEGF schemes differ substantially as far as formalism and implementation are concerned, they give practically indistinguishable results. This is not surprising, having in mind that the continuum Dirac picture is the effective theory corresponding to the low energy tight-binding method. Therefore, both approaches display these Zeeman-like effects, even though we use only minimal coupling and the Peierls substitution respectively, to account for the influence of the magnetic field. However, unlike the orbital moments coupled to the spin, the valley-contrasting orbital moments can not be captured by the TB NEGF transport simulations, since the contributions from the two valleys are inherently summed over. In this case, only the continuum calculations, where the valley degree of freedom is explicit, can capture the relevant physics.

VI. CONCLUSION

In this paper we have shown that in Dirac systems in which spin-orbit coupling is prominent, such as silicene, germanene, stanene or functionalized graphene, orbital magnetic moments coupled to the spin degree of freedom will arise, thus leading to the renormalization of the g-factor. These moments appear due to the self-rotation of the wavepackets in the vicinity of the two valleys, and reflect the topology of the band structure. They are entirely analogous to the valley-contrasting orbital moments found in honeycomb lattices with broken spatial symmetry, with whom they share a similar functional form. Therefore, the duality between \( \Delta_{SO} \) and the spin quantum number on one hand, and \( \Delta \) and the valley quantum number on the other hand is established. It is also shown that this duality reflects on the zeroth Landau levels, once the perpendicular magnetic field is applied.

To explore the influence of the orbital magnetic moments on the transport properties, we have studied the transmission through a single 1D barrier made of artificially enhanced spin-orbit coupling in graphene. We have shown that certain magneto-transport signatures are a clear manifestation of the induced moments. In particular, the conductances \( G \) through the device for the two spins start deviating from each other with the increase of the magnetic field. However, the effects of the moments on the fringe pattern of the transmission coefficients are most clearly observed in the dependence of the conductance with respect to electron energy \( dG/dE \) on \( E \). This quantity reflects the growing shifts in the interference maxima of opposite spins with increasing magnetic field; they are largest near the band edges, and decrease for larger energies due to the decrease of the orbital magnetic moments themselves. Because of the analogy between the mass and the SOC terms and the orbital magnetic moments they induce, the results presented here are also valid for valley transmission through a massive barrier. This, however, can not be captured by numerical techniques such as the TB NEGF method, which is only able to account for the spin degree of freedom, and the associated orbital moments. In this case, the method could prove handy for studying the effects of disorder and imperfections on the manifestation of the orbital moments.

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Appendix A: Tight-binding nonequilibrium Green function method

The Green’s function of a system is given by

\[ G = (EI - H)^{-1}. \] (A1)

where \( H \) is the Hamiltonian of the entire structure. Here and in the rest of the Appendix we take the energy to be shifted infinitesimally along the imaginary axis, i.e. \( E \to (E + i\eta) \). This is the retarded Green function, the advanced one is obtained by simply taking the Hermitian conjugate. In the case of a system with two leads the tight binding Hamiltonian can be written as

\[ H = \begin{bmatrix} H_L & H_{LD} & 0 \\ H_{LD}^\dagger & H_D & H_{RD}^\dagger \\ 0 & H_{RD} & H_R \end{bmatrix}. \] (A2)

The only finite matrix here is the device Hamiltonian \( H_D \), while all other matrices are infinite in size. \( H_L \) describes the hopping in the left lead, \( H_R \) describes the hopping in the right lead, \( H_{LD} \) and \( H_{RD} \) describe the hopping from the device to the left lead, and from the device to
the right lead respectively, while their Hermitian adjoints describe the hopping in the reverse direction.

The corresponding Green function is likewise represented via submatrix blocks

\[ G = \begin{bmatrix} G_L & G_{LD} & G_{LR} \\ G_{DL} & G_D & G_{DR} \\ G_{RL} & G_{RD} & G_R \end{bmatrix}. \]  

(A3)

Having in mind the definition of the Green function, Eq. (A1), one can arrive at the following set of equations

\[ (E - H_L)G_{LD} + H_{LD}G_D = 0, \]
\[ H_{LD}^\dagger G_{LD} + (E - H_D)G_D + H_{DR}G_{RD} = I, \]  

(A4)

\[ H_{DR}^\dagger G_D + (E - H_R)G_{RD} = 0. \]

After some manipulation one obtains

\[ G_D = (E - H_D - \Sigma_L - \Sigma_R)^{-1}, \]  

(A5)

where \( \Sigma_L = H_{LD}^\dagger g_L H_{LD} \) and \( \Sigma_R = H_{RD}^\dagger g_R H_{RD} \) are the effective self-energy terms appearing in the Green function of the device due to the semi-infinite left and right leads, and \( g_{L/R} = (E - H_{L/R})^{-1} \) are their respective Green functions. In order to obtain these functions we employ the scheme laid out in Ref. [36]. The benefit of self energy matrices is that they are finite, thanks to the fact that the semi-infinite leads connect via hopping elements only to the surface sites in the device. Therefore it can be said that in this procedure the leads are integrated out of the problem, since we are left with the finite-sized Green function of the device itself. It is important to point out that incorporating the influence of the infinite leads through the finite self-energy matrices is exact.

Once these and the broadening matrices \( \Gamma_{L/R} = i \left( \Sigma_{L/R} - \Sigma_{L/R}^\dagger \right) \), are obtained, the transmission through the structure can be calculated as

\[ T = Tr \left( \Gamma_L G_D^\dagger \Gamma_R G_D \right). \]  

(A6)

In order to compare the results with the continuum theory, we need the numerical simulations within the NEGF formalism to provide us with angular dependence of the transmission through a structure infinite in the \( y \) direction. To achieve this, we resort to the recipe described in Ref. 37. In short, we take the smallest possible zigzag nanoribbon, placed along the \( x \) direction, where the semi-infinite left and right leads surround the barrier region in which SOC NNN hopping is nonzero. The structure is then taken to be periodic along the \( y \) direction, prompting the use of the Bloch theorem in this direction. This means that the phase factor will enter all hopping terms along the \( y \) axis, which is non other than the transverse momentum \( k_y \). In this way, \( k_y \) appears as a parameter, and since the incident energy \( E \) is a parameter as well, one is then able to reconstruct the angle of propagation using \( h v_F k_y = E \sin \phi \). Note that in our case, besides the Peierls phase factor, we also must add the vector potential, Eq. (19) to \( k_y \), in order to properly model the influence of the magnetic field. Finally, one needs to connect the Fermi velocity \( v_F \) entering the Dirac equation, with the nearest-neighbor hopping \( t \), as \( v_F = 3a/2h \), where \( a = 0.142 \text{ nm} \) is the carbon-carbon distance, and the hopping is set to \( t = 2.7 \text{ eV} \)
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