Spin Orbit Interaction and Isotropic Electronic Transport in Graphene

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Broken symmetries in graphene affect the massless nature of its charge carriers. We present an analysis of scattering by defects in graphene in the presence of spin-orbit interactions (SOIs). A characteristic constant ratio (≥2) of the transport to elastic times for massless electrons signals the anisotropy of the scattering. We show that SOIs lead to a drastic decrease of this ratio, especially at low carrier concentrations, while the scattering becomes increasingly isotropic. As the strength of the SOI determines the energy (carrier concentration) where this drop is more evident, this effect could help evaluate these interactions through transport measurements.

PACS numbers: 72.10.Fk, 75.76.+j, 72.80.Vp, 03.65.Pm

The discovery of graphene has stimulated numerous theoretical and experimental works [1], opening new doors for promising new technology due to its low dimensionality and high carrier mobility. The low energy electron dynamics is described by two inequivalent points at the Brillouin zone (K and K’) known as Dirac points, since the linear dispersion is equivalent to two-dimensional massless Dirac fermions [2, 3].

The importance of graphene on transport devices also motivates the identification and understanding of spin dynamics [4], as an important element in the development of spintronics. In graphene, interface or bulk broken symmetries allow for the existence of two kinds of spin orbit interaction (SOIs) that affect spin dynamics in different ways [5]. The hexagonal arrangement of carbon atoms allows an intrinsic SOI that respects lattice symmetries and can be seen to arise from the atomic SO coupling. This generates a gap in the spectrum, a mass term in the Dirac equation with sign depending on the spin, pseudospin and Dirac valley [6, 7]. An inversion asymmetry in graphene could also generate an extrinsic Rashba SOI, resulting from the effect of substrates, impurities generating sp² distortions such as hydrogen, fluorine or gold–perpendicular electric fields, or lattice corrugations [8–13]. Intercalation of gold under graphene deposited on nickel substrates results in very large Rashba interactions [13], while a large enhancement was observed in weakly hydrogenated samples [14]. In addition, recent theoretical studies have shown that decoration of graphene with heavy atoms such as indium and thallium will result in the enhancement of an intrinsic-like SOI in graphene and the associated quantum spin Hall state [15].

Adsorbed impurities [16, 17], as well as lattice vacancies and other local defects in the lattice [18], provide natural short-range scattering centers known as resonant scatterers. Sources of resonant scatterers are also organic groups [19], clusters of impurities [20], or even artificially controlled metallic islands deposited on the surface of graphene [21]. Extensive work has identified the existence of resonant scatterers as the main mechanism limiting carrier mobility in graphene samples [19–23]. These conclusions are supported by the insensitivity to screening effects provided by the different substrates used [24–25], by the independence of the ratio of the transport to elastic times to the carrier concentration [26], and by the universal presence of the Raman D peak in graphene devices and its stability after high-temperature annealing of samples [27, 28]. Experiments performed by Monteverde et al. [26] used the transport (τ_tr) and elastic (τ_e) scattering times extracted from magnetotransport measurements to probe the nature of the impurities in single and bilayer graphene. The ratio of these two characteristic times, ξ = τ_tr/τ_e, describes at low Fermi energies (low carrier concentration) the degree of angular anisotropy of the scattering process, offering an interesting insight on the type of impurities present in samples. One should comment that other work argues that carrier mobility in graphene is mainly limited by long range scattering from charged impurities [29, 32], also related to the formation of electron-hole puddles [2, 21, 30, 33].

Short range scatterers are categorized according to the total cross section, σ_t, they produce [26]: “Small cross section scatterers” have σ_t ∝ k, where k is the carrier Fermi wave number (k ∝ E_F ∝ √n_c, with n_c the carrier density). “Medium cross section scatterers” are referred in the literature also as resonant scatterers, and display a different dependence, σ_t ∝ 1/(k ln^2 k). Finally, the “large total cross section scatterers” or “unitary” are associated with the presence of a long-lived quasibound state [34, 35], and exhibit σ_t ∝ 1/k. An important common property shared by all these regimes is that the ratio of the transport to elastic times is determined fully by the conservation of pseudo-helicity, leading to a value of 2 at low energies, as we will discuss below.

We will show that the presence of SOIs leads to an important transformation of scattering processes in graphene, from highly anisotropic (zero backscattering) to more or fully isotropic at low energies, depending on...
the strength of these interactions. We show that the Rashba SOI results in the appearance of new unitary resonances for short-range scatterers, whenever Rashba coupling is comparable to the Fermi energy. Moreover, we show that the three different types of short range scatterers (off resonant, resonant, and unitary), lead to processes with different levels of angular isotropy, unlike the case with no Rashba SOI when all short range scatterers display similar anisotropy. These findings suggest that transport experiments performed at low carrier concentration could unveil the local enhancement of the Rashba interaction produced by impurities, lattice corrugations, or substrate effects, and provide a direct measurement of its strength.

We consider the presence of intrinsic SOI, affecting the carriers throughout the graphene system, while an extrinsic scatterer generates a local potential obstacle and corresponding Rashba SOI; the Hamiltonian for this system close to the Dirac points is then given by

\[ H = H_o + H_V + H_{SO} + H_R, \]

where \( H_o = \hbar v_F (\tau_z \sigma_x p_x + \sigma_y p_y) \) describes Dirac fermions in graphene, \( H_{SO} = \Delta_{SO} \sigma_z \tau_z s_z \) is the intrinsic SOI, \( H_V = V\Theta(R - r) \) is the scattering potential characterized by strength \( V \) over a region \( r < R \), and \( H_R = \lambda_R (\tau_x \sigma_x s_y - s_x \sigma_y) \Theta(R - r) \) is the Rashba SOI over the same region; here \( v_F \approx 6.6 eV/\text{A} \), while \( \sigma_x \) and \( s_\mu \) are Pauli matrices representing the electron pseudospin \((A, B)\) and spin \((\uparrow, \downarrow)\), respectively, and \( \tau_z = \pm 1 \) identifies the K or K' valleys. \( \Delta_{SO} \) and \( \lambda_R \) are the strengths of intrinsic and Rashba interactions, and \( \Theta \) is the Heaviside function. The characteristic size of the scatterers is assumed to be much larger than the lattice spacing in graphene for the continuum Dirac description of graphene to be appropriate, and to neglect intervalley scattering \[2, 36\].

The analytical form of the spinors \[37\] allows one to use a partial wave decomposition to study the scattering of an incoming flux of electrons along the \( x \)-direction \[38\], which takes the asymptotic form away from the scattering center

\[ \psi \approx e^{i k r \cos \theta} \chi_{in} + \hat{f}(\theta) \frac{e^{i k r}}{\sqrt{r}} \chi_{in}, \]

where \( \chi_{in} = (c_1 |\uparrow\rangle, c_2 |\downarrow\rangle)^T \) is a spinor describing the spin weights of the incoming flux with \( |\chi_{in}|^2 = 1 \), \( k = \sqrt{E^2 - \Delta_{SO}^2}/\hbar v_F \), and \( \hat{f}(\theta) \) is a matrix containing the different scattering amplitudes. The conservation of total angular momentum \( J_z = L_z + \hbar \tau_z \sigma_z/2 + \hbar s_z/2 \), where \( J_z \psi_n = \hbar n \psi_n \) \[37\], allows consideration of separate partial wave components of the incoming wave with a given spin \( s \), \( \psi_n^{(s)} \). Hence, the full wave function away from the scattering center is given by

\[ \psi_n^{\text{out}}(r, \theta) = \psi_n^{(s)}(s) + \sum_{s'} S_{n, ss'} \psi_n^{(s')}(s'), \]

where \( s, s' = \uparrow, \downarrow \) and \( \psi_n^{(s)} \) is an outwave. The asymptotic form of the Henkel functions and the Jacoby-Anger expansion \[37\], allows one to relate the wave functions in \[2\] and \[3\], and characterize the scattered part of the wave function as \( s = -s \)

\[ \psi_n^{\text{sc}} = \frac{e^{-i \pi/4}}{\sqrt{2\pi k}} \left( (S_{n, ss'} - 1) \psi_n^{(s')}(s) + i \bar{s} S_{n, ss'} \psi_n^{(s+)}(s) \right), \]

leading to the scattering amplitude matrix

\[ \hat{f}(\theta) = \frac{e^{-i \pi/4}}{i \sqrt{2\pi k}} \sum_n \begin{bmatrix} f_n^{\uparrow \uparrow} & f_n^{\uparrow \downarrow} \\ f_n^{\downarrow \uparrow} & f_n^{\downarrow \downarrow} \end{bmatrix} e^{i n \theta}, \]

where \( f_n^{ss'} = S_{n, ss'} - 1 \), \( f_n^{ss} = i \bar{s} S_{n, ss'} \), and the sum over \( n \) in \( \hat{f}(\theta) \) runs over all integers. Conservation of flux for each channel of angular momentum (unitarity of \( S \)), imposes the condition \( |S_{n, ss'}|^2 + |S_{n, s\tilde{s}}|^2 = 1 \), so that one can relate the scattering amplitudes to the phase shifts gained during the scattering process by \( S_{n, ss'} = e^{i \delta_{s\tilde{s}} \varphi} \cos \delta_{n, ss'} \) and \( S_{n, s\tilde{s}} \equiv \sin \delta_{n, ss'} \), where \( \delta_{n, ss} \) is the phase for spin preserving processes and \( \delta_{n, s\tilde{s}} \) is conveniently defined for spin-flipping events \[39, 41\]. The description above, an extension of the partial wave component method \[38\], allows for the exploration of spin-dependent phenomena \[39\] and observables such as: the differential cross section \( \sigma(\theta) \), that explicitly displays the anisotropy of the scattering; the transport cross section \( \sigma_T \), related to the transport mean free time, \( \sigma_T = n_{imp} v_F \sigma_T \); and the total cross section \( \sigma_T \), related to the elastic scattering time, \( \sigma_T^{-1} = n_{imp} v_F \sigma_T \), where \( n_{imp} \) is the impurity concentration in the sample. In the presence of SOIs the scattering includes spin-preserving and spin-flip events. Correspondingly, all these cross sections are spin-dependent matrices given by

\[ \sigma_{ss'}(\theta) = \frac{1}{2\pi k} \left| \sum_n f_n^{ss'} e^{in\theta} \right|^2, \]

\[ \sigma_{tt'} = \frac{1}{k} \sum_n |f_n^{ss'}|^2, \]

and

\[ \sigma_{tr, ss'} = \sigma_{tt', ss'} - \frac{1}{k} \sum_n \Re \left( f_n^{ss'} f_{n+1, ss'}^* \right). \]

In the absence of SOIs the pseudo-helicity, \( \sigma \cdot p/p \) is a conserved quantity \[2, 38\] and results in the equality

\[ f_m = f_{-(m-1)}, \]

where \( m \) is an integer \( (m = m \mp \frac{1}{2} \text{ for } \uparrow / \downarrow) \) \[37, 38\], which leads to a vanishing differential cross section at \( \theta = \pi \) (Klein tunneling), \( \sigma(\theta = \pi) = 0 \), indicating the anisotropic character of the scattering process and the near transparency of barriers in graphene \[12, 43\]. At low carrier concentrations, \( kR \ll 1, f_0 \equiv f_1 \)
and $f_{m\neq0,1} \approx (kR)^m$, leading to $\sigma_{\uparrow} \approx 2\sigma_{\tau \tau}$, and therefore $\xi = \tau_{\tau}/\tau_{\tau} \approx 2$.
Therefore, scattering of massless Dirac fermions in graphene from short range potential scatterers results in $\xi \approx 2$, for all $V$ and $R$, as long as the carrier density is small, $kR \ll 1$.

This ratio is fully determined by the number and equal weights of the angular momentum channels contributing to the scattering process. As we will see below, this situation is drastically changed in the presence of SOI.

**Graphene with intrinsic SOI.** Graphene systems with uniform intrinsic SOI (for space dependent $\Delta_{SO}$ see [38]), $\Delta_{SO} \neq 0$, represent a rich opportunity to explore topological effects. An example of such a system is predicted by appropriate deposition of heavy metal atoms on graphene [15]. In those cases, the eigenstates no longer have a well-defined pseudo-helicity, due to the carrier mass generated by the SOI; notice however that although this mass is spin-dependent, it does not cause intravalley spin-flip processes, and the scattering can still be analyzed in terms of independent spins. The broken pseudo-helicity, however, results in $\delta_{n,ss} \neq \delta_{-(n-1),ss}$. However, effective time reversal symmetry [40] imposes the relations $f_{n,ss} = f_{-n,ss}$, and $f_{n,ss} = f_{-n,ss}$, and since spin mixing is not produced by the intrinsic SOI, we have $\delta_{n,ss} = \delta_{-(n-1),ss}$.

As one could suspect, the isotropy of the scattering process depends on the ratio of $\Delta_{SO}/E$, as shown in Fig. 1 the scattering is anisotropic—with absence of back scattering—for $\Delta_{SO} = 0$, while it becomes increasingly isotropic with larger $\Delta_{SO}/E$, and for $\Delta_{SO} \approx E$, the scattering is equally probable in all directions.

The change in the isotropy of the scattering process is related to the total number of angular momentum channels contributing to the cross section. For an incoming electron flux with “high” energy, $0 \leq \Delta_{SO}/E \ll 1$, the system exhibits approximately equal contributions from two scattering channels, $n = 0$ and $n = 1$ for $\uparrow$ incoming flux (or $n = 0$ and $n = -1$ for $\downarrow$ incident flux), and these contributions satisfy $f_{0,\uparrow\uparrow} \approx f_{1,\uparrow\downarrow}$ (or $f_{0,\downarrow\downarrow} \approx f_{1,\downarrow\uparrow}$). In contrast, we observe an increase in the isotropy of the scattering as $E$ decreases, approaching $\Delta_{SO}$, due to the vanishing contribution of the $n = 0$ channel to the total cross section, $\sigma(kR^2, \tau/E)$, compared to resonant contribution of the $n = \pm 1$ channels $\pi^2/(k\ln^2(kR))$ [37]. This leads to the “isotropic” ratio of $\xi = \tau_{\tau}/\tau_{\tau} \approx 1$, which is characteristic of the scattering of massive particles at low energies; in other words, one of the spinor components dominates the scattering process in this range of energy and leads to a fully isotropic differential scattering cross section. As $\Delta_{SO}$ determines the energy scale for which the isotropy would play a larger role, the exploration of decorated graphene samples would be an interesting system in which to test these results [15].

**Graphene with Rashba SOI.** We now analyze the case of graphene samples containing scattering centers that also produce Rashba interactions [9, 10, 13, 14]. $\Delta_{SO} \ll \lambda_{R} \neq 0$ [37], allowing spin flip events. This requires a detailed analysis of the spin dependent scattering processes. When $kR \ll 1$, we have two contributing channels, depending on the spin of the incoming particle ($n = 0$ for spin up, and $n = 0, -1$ for spin down), similar to the case discussed above for $\Delta_{SO} \neq 0$. Effective time reversal symmetry within the Dirac cone allows one to study the scattering of a given spin without loss of generality [37, 40].

Curves of total cross section vs. scattering potential strength $V$ are shown in Fig. 2 for $kR \ll 1$, and different values of the Rashba SOI interaction, $\lambda_{R}$; analytical expressions for the different contributions can be obtained as well [37]. Figure 2 shows how the location and number of resonances change in the presence of Rashba SOIs. The resonances at $\chi = \chi_{0} \pm \lambda_{R}kR/\hbar v_{F}$ for both $\sigma_{\uparrow\uparrow}$ and $\sigma_{\uparrow\downarrow}$, can be identified as resonances of the $n = 0$ chan-
while the resonance at \( \chi \) of Rashba coupling for different energies. A clear drop of coupling and \( V \) in the range of 5 Å ≤ \( R \) ≤ 8 Å, not unlike those considered before [9, 26].

\[ 5 \text{ to } 8 \text{ Å} \]

Fig. 3, where the results of such averaging procedure are shown. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed. Notice that the range of \( \xi \) values is different from the case of no SOI, by showing that the ratio \( \xi_R \) is kept fixed.
