THERMOPOWER OF A GRAPHENE MONOLAYER WITH INHOMOGENEOUS SPIN-ORBIT INTERACTION

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ABSTRACT. We consider a single layer of graphene with a Rashba spin-orbit coupling localized in the central region. Generally, a spin-orbit interaction induces a spin splitting and modifies the band structure of graphene, opening a gap between the two sublattices. We investigate the transport properties within the scattering approach and calculate the linear electric and thermoelectric conductances. We observe a weak dependence of the electric conductance with both the length of the spin-orbit region and the Rashba strength. Strikingly, the thermoelectric conductance is much more sensitive to variations of these two parameters. Our results are relevant in view of recent developments that emphasize thermoelectric effects in graphene.

1. Introduction. The considerable interest in graphene, a purely two-dimensional crystal, is partly due to its peculiar electronic properties [1]. The energy spectrum is described with conduction and valence bands that touch each other at six different points, which are reduced to two (\(K\) and \(K'\)) for symmetry reasons. At low energies, the energy band structure near \(K\) and \(K'\) becomes two cones that come into contact at their vertices. Thus, long-wavelength electrons behave as massless fermions traveling at fixed velocity \(V_F \sim 10^6\) m/s and their low-energy excitations are accounted for with an effective Dirac equation where the speed of light is replaced by \(V_F\).

In Ref. [2], we investigated the electric and thermoelectric properties of graphene under the influence of local Rashba spin-orbit interaction [3]. The subject is interesting because recent studies suggest enhanced thermopowers in graphene monolayers and nanoribbons [4, 5, 6, 7]. Very recently, thermoelectrically generated photocurrents have been detected in p-n junctions [8, 9]. We found that the Seebeck coefficient, which measures the voltage generated in response to an applied thermal gradient, exhibits an intrinsic contribution that is independent of the sample details. In contrast, the thermoelectric conductance shows oscillations as a function of the Fermi energy. However, for an accurate characterization of the thermoelectric properties of spin-orbit graphene it is important to analyze the transport coefficients as a function of the length of the Rashba region and its coupling strength. This is the goal we want to accomplish here.

2. Model. We consider a graphene monolayer in the \(xy\) plane. The Hamiltonian in the continuum limit near the Dirac points reads

\[
\mathcal{H} = -i\hbar V_F (\sigma_x \partial_x + \sigma_y \partial_y) \otimes s_o + \lambda (\sigma_x \otimes s_y - \sigma_y \otimes s_x).
\]  

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Figure 1. Energy spectrum of our spin-orbit graphene device. In the left and right sides, we show the energy band structure of a bare graphene sheet. In the central region, energy bands are split due to the Rashba coupling. Solid lines indicate propagating states while dashed lines depict evanescent states.

The first term is the Hamiltonian for a clean graphene sheet. \( s \) and \( \sigma \) are Pauli matrices in the spin and pseudospin (sublattice) spaces, respectively. This model is valid when intervalley scattering can be safely neglected. The second term introduces the Rashba spin-orbit coupling and \( \lambda \) is the parameter of this interaction. For the continuum model to remain valid, we assume that \( \lambda \) is a slowly varying function in a length scale larger than the lattice constant. Interestingly, \( \lambda \) can be externally tuned with doping or electric fields. In fact, relatively strong Rashba strengths have been observed in graphene deposited onto metallic substrates [10, 11]. In what follows, we take nonzero \( \lambda \) for \( 0 < x < L \) and zero otherwise.

We take \( k(q) \) as the momentum in the \( x(y) \) direction. Then, the eigenstates of our Hamiltonian are

\[
E_{l,n} = \pm \sqrt{\lambda^2 + \hbar^2 V_F^2(k^2 + q^2) + n\lambda},
\]

where \( l = \pm \) labels states with positive or negative energies and \( n = \pm \) is the subband index. For \( \lambda = 0 \) we recover the linear spectrum of bare graphene, as depicted in the left and right sides of Fig. 1. For a nonzero value of \( \lambda \) the spectrum splits into four bands with a parabolic dependence on \( k \), see the solid lines in the central region of Fig. 1. The band splitting is given by the Rashba strength \( 2\lambda \).

The eigenstates of \( \mathcal{H} \) are

\[
\psi_{l,n}^m(x) = \frac{e^{imkx}e^{iqy}/2}{\sqrt{\hbar^2 V_F^2(k^2 + q^2) + E_{l,n}^2}} \begin{pmatrix}
-E_iV_F(mk - iq) \\
E_{l,n}
\end{pmatrix},
\]

where \( m = \pm \) indicate the propagation direction, which determines the sign of the momentum along \( x \). Since our problem is invariant along the \( y \) direction, the \( q \) momentum component is conserved during any scattering event. However, \( k \) can become purely imaginary for spatially localized states, as those depicted with dashed lines in Fig. 1. To analyze the scattering induced by the local spin-orbit field, the asymptotic states at \( x \rightarrow \pm \infty \) are taken as propagating (i.e., real \( k \)) but in the central region we allow for both propagating and evanescent states.
For completeness, we also write down the $\lambda = 0$ dispersion relation,

$$E_l = \hbar V_F \sqrt{k^2 + q^2},$$  \hspace{1cm} (4)

with associated eigenstates

$$\psi_{l,n}^m(x,y) = \frac{e^{imkx}e^{iqy}}{2} \begin{pmatrix} -ine^{-im\phi} \\ l \\ -inl \\ me^{im\phi} \end{pmatrix}.$$  \hspace{1cm} (5)

Here, $\phi$ is the wavevector angle defined as $\phi = \tan^{-1} q/k$. The left and right sides of Fig. 1 are calculated for $q = 0$. Then, the spectrum $E(k)$ has a slope proportional to $V_F$.

3. **Scattering Approach.** We consider three regions, as shown in Fig. 2: the left and right sides are bare graphene whereas the central region of length $L$ is subjected to Rashba spin-orbit coupling, with $x$ the transport direction. Because the spin-orbit interaction is inhomogeneous along $x$, the $y$ component of the momentum can be fixed in terms of the wavevector angle, $q = \frac{E}{\hbar V_F} \sin \phi$. We take the width $W$ along the $y$ direction as a large dimension to avoid edge effects.

Our system shows particle-hole symmetry, even in the presence of Rashba coupling. Therefore, it suffices to study the case $E > 0$. To find the $k$ momentum in the side regions, $x < 0$ and $x > L$, we use Eq. (4)

$$k = E\sqrt{(1 - \sin^2 \phi)/hV_F}.$$  \hspace{1cm} (6)

For the central region, $0 < x < L$, the wavevector component parallel to the transport direction is determined from Eq. (2):

$$k^n = \sqrt{E(E - 2n\lambda - E\sin^2 \phi)/hV_F}.$$  \hspace{1cm} (7)

In this region we have two possibilities for $k^n$, one per each branch ($n = \pm$). When we analyze more closely this dependence with $n$, we infer that the momentum will be real for any energy if $E - 2n\lambda - E\sin^2 \phi > 0$, i.e.,

$$\sin \phi < \sqrt{\frac{E - 2n\lambda}{E}}.$$  \hspace{1cm} (8)

For $n = -$ this relation is always true independently of the value of the energy since $\sin \phi$ is bounded. However, for $n = +$ and $E > 2\lambda$ we have a critical angle for which the momentum
is purely imaginary and the electron wave becomes evanescent. Instead, for $0 < E < 2\lambda$ this relation is never satisfied and the wave is always evanescent for any value of $\phi$. This critical angle effect can be explained as a total internal reflection phenomenon.

To solve the scattering problem sketched in Fig. 2, we express the wave function at each region as $\psi_{m,n}^r(x,y) = \psi_n^m e^{ikx} e^{iqy}$ [cf. Eq. (3)]. We first specify left ($l$) wave function for $x < 0$:

$$\psi_{l,n}(x,y) = \psi_n^+ e^{ikx} e^{iqy} + r_{n,-} \psi_n^- e^{-ikx} e^{iqy} + r_{n,+} \psi_n^+ e^{-ikx} e^{iqy},$$

(9)

where the incident subband $n$ can be taken as $+$ or $-$ because the bands in this region are doubly degenerate. Equation (9) describes an incident wave with positive group velocity and two reflected waves into the $-$ and $+$ modes, with negative velocity, and reflection amplitudes $r_{n,-}$ and $r_{n,+}$, respectively. In the central ($c$) the wave function has four components,

$$\psi_{c,n}(x,y) = a_{n,-} \psi_n^+ e^{ikx} e^{iqy} + b_{n,+} \psi_n^+ e^{ikx} e^{iqy} + c_{n,-} \psi_n^- e^{-ikx} e^{iqy}$$

$$+ d_{n,+} \psi_n^- e^{-ikx} e^{iqy},$$

(10)

where the coefficients $a$, $b$, $c$, and $d$ are labeled with the incident subband $n$ and the reflected or transmitted index in the central region. Equation (10) is valid for $E > \lambda$. For $0 < E < \lambda$ one must consider the evanescent states emerging from the $E < 0$ spectrum, as seen in Fig. 1 (dashed cyan line). Finally, in the right ($r$) region we only have transmitted waves with positive group velocity and positive and negative $n$:

$$\psi_{r,n}(x,y) = t_{n,-} \psi_n^+ e^{ikx} e^{iqy} + t_{n,+} \psi_n^+ e^{ikx} e^{iqy},$$

(11)

where $t_{n,\pm}$ is the transmission amplitude from the $n$-th incident subband toward the $\pm$ mode.

Since the Hamiltonian is first order in the momentum, it is enough to invoke the continuity of the wave function in the potential discontinuities, $x = 0$ and $x = L$:

$$\psi_{l,n}(0,y) = \psi_{c,n}(0,y),$$

(12)

$$\psi_{r,n}(L,y) = \psi_{r,n}(L,y),$$

(13)

from which we determine the eight coefficients $r_{n,\pm}$, $a_{n,-}$, $b_{n,+}$, $c_{n,-}$, $d_{n,+}$ and $t_{n,\pm}$.

Current conservation demands that reflection and transmission processes are connected via

$$1 = R_{n,+} + R_{n,-} = T_{n,+} + T_{n,-},$$

(14)

where $R_{n,\pm} = |t_{n,\pm}|^2$ ($T_{n,\pm} = |t_{n,\pm}|^2$) is the probability that an electron with subband index $n$ be reflected (transmitted) with subband index $\pm$. In the following, we focus on the diagonal components $T_{n,+}$ and $T_{n,-}$ since the off-diagonal transmissions, $T_{n,-}$ and $T_{n,+}$, vanish due to the spin-chiral nature of electrons in graphene.

4. Electric conductance. The electric current of electrons in the subband $n$ is obtained from transmission probability integrated over all possible states with energy $E$ and incident angle $\phi$,

$$I_n = \frac{2eW}{\pi h} \int_0^{\pi/2} \cos \phi \, d\phi \int_{-\infty}^{\infty} K(E) T_{n,n}(E, \phi) [f_s(E) - f_r(E)] \, dE,$$

(15)

where $f_s(E)$ and $f_r(E)$ are Fermi-Dirac distribution functions accounting for the thermal population of electrons in the coupled reservoirs. In Eq. (15) $K(E) = E / h\nu_F$ is obtained from the graphene dispersion relation, Eq. (4). The total current is thus $I = \sum_n I_n$.

We are interested in small deviations from equilibrium. The conductance at linear response is thus $G = (dI/dV)_{V=0}$ where $V$ is the voltage bias across the junction. We take the left Fermi-Dirac factor as $f_s = f(E - eV)$ and the right one as $f_r = f(E)$, where
$f(E) = \frac{1}{1 + e^{(E-E_F)/k_B T_0}}$ is the equilibrium distribution function with $E_F$ the Fermi energy and $T_0$ the background temperature. At $T_0 = 0$, we find

$$G_n = G_0 \int_0^{\pi/2} T_{n,n}(E_F, \phi) \cos \phi d\phi,$$

(16)

where $G_0 = 2e^2Wk_F/\pi \hbar = 4e^2W{E_F}/h^2V_F$ is the maximum conductance of an ideal two-dimensional conductor since $\text{Int}(Wk_F/\pi)$ is the number of open channels of a sample with Fermi wave number $k_F$. Hence, the total electric conductance is $G = \sum_n G_n$.

The transmission probability, and therefore the conductance, depends on the length of the central region, $L$, and the parameter of the Rashba coupling, $\lambda$. In Fig. 3 we show the electric conductance, $G$, as a function of $L$ (left side) and $\lambda$ (right side) for a fixed Fermi energy. In Fig. 3(a) both $G_+$ and the $G_-$ are trivially equal to unity if $L = 0$ because the wave is completely transmitted. When $L$ increases, we observe that $G_+$ decreases quickly. This is due to the fact that we are considering the case $E_F < 2\lambda$, for which the states in the central region are evanescent [see red dashed line in Fig. 1]. The transmitted part is due to electron tunneling, with a probability that quickly decreases as $L$ increases and becomes negligible for long spin-orbit regions. On the contrary, the electric conductance with negative subband index, $G_-$, is always close to unity since the wave functions corresponding to $E_+ < 2\lambda$ [see magenta solid line in Fig. 1] are propagating states for any incident energy $E > 0$. Our conclusion is reinforced by the oscillations seen in $G_-$, which typically arise in scattering problems with wave interference even for energies above the potential threshold.

In Fig. 3(b) we observe a similar behavior but in this case the nonzero part of $G_+$ is mainly due to states with $E_F > 2\lambda$, which are propagating. The transition is not abrupt since, although the states for $E_F < 2\lambda$ are evanescent, they also contribute to transmission via tunneling. Independently of the value of $\lambda$ the conductance term $G_-$ is close to one because there always exists an available channel for any $\lambda > 0$.

Clearly, our results show that either by tuning the spin-orbit region length or strength, a subband polarization of the outgoing electronic states can be achieved for large values of $L$ or $\lambda$. To quantify this effect we define the subband polarization as

$$P = \frac{G_+ - G_-}{G_+ + G_-},$$

(17)

We represent $P$ in Fig. 4 as a function of $L$ (left) and $\lambda$ (right). Figure 4(a) shows that at low $L$ the electron wave is nonpolarized because the tunneling probability is close to one for small $L$. As we increase the width of the central region, less waves with $n = +$ are transmitted and the outgoing wave is negatively polarized. Figure 4(b) presents the
subband polarization as a function of Rashba coupling strength for fixed $E_F$ and $L$. When $\lambda$ is small the outgoing wave is not polarized because we have propagating states for each subband index ($E_F > 2\lambda$). As we increase $\lambda$ the states with positive $n$ becomes evanescent inside the central region and the transmission probability is vanishingly small. Thus, for $E_F > 2\lambda$ most electrons have negative polarization.

5. Thermoelectric conductance. The thermoelectric conductance is obtained from the current generated in the linear response regime for a small temperature shift $\Delta T$ applied across the sample. In Eq. (15) we replace the left Fermi-Dirac function with $f(E, T_0 + \Delta T)$ and the right one with $f(E, T_0)$. The leading-order Taylor expansion reads,

$$ I_n = \frac{2eW}{\hbar \pi} \int_0^{\pi/2} \cos \phi \, d\phi \int \frac{E}{\hbar V_F}(E - E_F) \left( \frac{\partial f}{\partial E} \right) T_{n,n}(E, \phi) \, dE. \quad (18) $$

For zero temperature the thermocurrent is zero ($I_n = 0$). To find the leading-order nonzero response, we use a Sommerfeld expansion,

$$ \int_{-\infty}^{\infty} H(E) \left( -\frac{\partial f}{\partial E} \right) \, dE \simeq \sum_{m=1}^{\infty} a_m (K_B T)^{2m} H^{(2m)}(E)|_{E=E_F}, \quad (19) $$

with $H(E) = E(E - E_F) \sum_n T_{n,n}^0(E, \phi)$ and $a_m = 2 \sum_{\nu=1}^{\infty} \frac{(-1)^{\nu+1}}{\nu^m}$. The thermoelectric conductance is $\mathcal{L} = I/\Delta T = \sum_n \mathcal{L}_n$, where

$$ \mathcal{L}_n = \mathcal{L}_0 \left[ \int_0^{\pi/2} T_{n,n}(E_F, \phi) \cos \phi \, d\phi + E_F \frac{\partial}{\partial E_F} \int_0^{\pi/2} T_{n,n}(E_F, \phi) \cos \phi \, d\phi \right]. \quad (20) $$

Here, we have defined $\mathcal{L}_0 = k_B^2 e WT_0/3\hbar^2 V_F$.

In Fig. 5 we show the thermoelectric conductance as a function of $L$ (left side) and $\lambda$ (right side). On the left side we represent $\mathcal{L}(L)$ for fixed Fermi energy and Rashba strength. At zero $L$ we find that the two components of $\mathcal{L}$ are close to unity since all electrons are transmitted. For larger $L$, $\mathcal{L}_+$ slowly decreases to zero. The effect is similar to the conductance discussed above: for $E < 2\lambda$ the states with $n = +$ are transmitted solely by conventional tunneling. As expected, the thermoelectric conductance with $n = -$ is larger because the states with $n = -$ are propagating but we also observe a strong variation with the central region length. $\mathcal{L}(\lambda)$, see the right side of Fig. 5, shows a strong dependence with the value of the Rashba strength. Interestingly, when we increase $\lambda$ sufficiently we can even obtain a negative thermoelectric conductance for a fixed $L$ and $E_F$. This means that for those high values of the Rashba strength electrons will travel from the cold to the hot.

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**Figure 4.** (Color online) Left: Subband polarization as a function of $L$. Parameters: $E_F = 15$ meV and $\lambda = 10$ meV. Right: Subband polarization as a function of $\lambda$. Parameters: $E_F = 30$ meV and $L = 100$ nm.
Figure 5. (Color online) Left: Thermoelectric conductance as a function of \( L \). Parameters: \( E_F = 15 \text{ meV} \) and \( \lambda = 10 \text{ meV} \). Right: Thermoelectric conductance as a function of \( \lambda \). Parameters: \( E_F = 30 \text{ meV} \) and \( L = 100 \text{ nm} \).

These strong variations are a consequence of the dependence of \( \mathcal{L} \) on the transmission derivative unlike the conductance, which depends on the transmission only.

In general, thermoelectric effects are analyzed in terms of the Seebeck effect, which takes into account the generation of a thermovoltage in an open-circuit conductor when a temperature bias is applied. Importantly, our system shows two subbands due to the spin-orbit interaction. Then, we consider a different chemical potential \( \mu_{\alpha n} = E_F + eV_n \) for each energy branch, where \( \alpha = \ell, r \). In each side of the junction we have a different temperature \( T_{\alpha} \) independently of the subband index \( n \). However, we allow for different populations (i.e., different electrochemical potentials) in opposite subbands. Then, we calculate the current due to a small shift in temperature, \( T_\ell - T_r \) and in voltage \( \mu_\ell n - \mu_r n \).

\[
I_n = \frac{\mu_\ell n - \mu_r n}{e} G_n + (T_\ell - T_r) \mathcal{L}_n , \tag{21}
\]

where the transport coefficients \( G_n \) and \( \mathcal{L}_n \) are given by Eqs. (16) and (20), respectively. We define

\[
\Delta T = T_\ell - T_r \tag{22a}
\]

\[
\mu_\alpha = \frac{1}{2}(\mu_{\alpha +} + \mu_{\alpha -}) \tag{22b}
\]

\[
eV = \mu_\ell - \mu_r \tag{22c}
\]

\[
eV_s = (\mu_{\ell +} - \mu_{\ell -}) - (\mu_{r +} - \mu_{r -}) \tag{22d}
\]

where \( V_s \) the subband voltage, which carries information about the possible population imbalances in different subbands. Using Eq. (22) in Eq. (21), we find the total current

\[
I = (G_+ + G_-) V_s + \frac{1}{2}(G_+ - G_-) V_s + (\mathcal{L}_+ + \mathcal{L}_-) \Delta T , \tag{23}
\]

and the subband current \( I_s = I_+ - I_- \),

\[
I_s = (G_+ - G_-) V_s + \frac{1}{2}(G_+ + G_-) V_s + (\mathcal{L}_+ - \mathcal{L}_-) \Delta T . \tag{24}
\]

In Eqs. (23) and (24), the transport coefficients are given by Eqs. (16) and (20). The subband current, Eq. (24) is akin to a spin current but in the subband space.

To simplify the notation we define the integrated transmission per subband as

\[
\mathcal{T}_n(E_F) = \int_0^{\pi/2} T_n,E_F,\phi \cos \phi d\phi . \tag{25}
\]
Then Eqs. (16) and (20) can be written in the following form

\[ G_n = \left( \frac{e}{\pi \hbar} \right)^2 \frac{W E_F}{V_F} T_n(E_F), \]  

\[ \mathcal{L}_n = \frac{e k_B^2}{3 \hbar^2} \frac{W T_0}{V_F} \left[ T_n(E_F) + E_F \frac{\partial T_n}{\partial E_F} \right], \]

where \( \frac{\partial T_n}{\partial E_F} \) is the energy derivative of \( T_n \) evaluated at \( E_F \).

The Seebeck coefficient or thermopower \( S = \frac{V}{\Delta T} \) takes the following form:

\[ S = -\frac{1}{2} \left( \frac{\mathcal{L}_+}{G_+} + \frac{\mathcal{L}_-}{G_-} \right). \]

Introducing Eqs. (26) in Eq. (27), we obtain the low-temperature thermopower

\[ S = -\frac{\pi^2 k_B}{3e} \frac{k_B T_0}{E_F} \left( 1 + E_F \frac{\sum \frac{\partial T_n}{\partial E_F}}{\sum T_n} \right). \]

We can observe two contributions in Eq. (28). The second term is a transport contribution, \( S_{tr} \), that can be explained with the Mott formula [12], \( S \propto \ln G/\partial E_F \). Surprisingly, we obtain an additional term which is independent of the spin-orbit interaction, \( S_m \). This is an intrinsic contribution which is independent of the sample characteristics and is nonzero even if the transmission weakly depends on energy [2].

In Fig. 6 we present the Seebeck coefficient as a function of \( L \) (left side) and \( \lambda \) (right side). In both cases the intrinsic part of the thermopower is constant since the Fermi energy is a fixed parameter. In Fig. 6(a) we observe that \( S(L) \) never changes sign because \( \lambda \), which controls this effect, is fixed. However, we observe a strong modulation of the thermopower with \( L \), which may serve as a useful tool for tuning \( S \) in a graphene layer. In Fig. 6(b) we show \( S(\lambda) \), which can now change sign as a function of \( \lambda \). Therefore, the generated voltage can be tuned with the Rashba strength.

6. Conclusions. We have analyzed the transport properties of a graphene layer in the presence of inhomogenous spin-orbit interaction. We have found that the linear conductance is dominated by a given energy subband for large enough spin-orbit strengths or region sizes. Interestingly, we have found a strongly modulated thermoelectric conductance as a function of both parameters, which suggests useful applications of spin-orbit graphene as a heat-to-energy converter. Despite the fact that the Seebeck coefficient always shows an intrinsic term independent of the scattering details, we have also obtained highly tunable thermopowers as a function of the Rashba coupling and the width of the spin-orbit...
region. In general, our system is more sensitive to temperature biases than voltage differences. Future works should investigate the validity of this statement for nanoribbons [13], magnetic samples [14] or different spin-orbit two-dimensional systems such as silicene [15] and semiconductor heterostructures [16].

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