Intrinsic contribution to spin Hall and spin Nernst effects in a bilayer graphene

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Abstract
We consider intrinsic contributions to the spin Hall and spin Nernst effects in a bilayer graphene. The relevant electronic spectrum is obtained from the tight binding Hamiltonian, which also includes the intrinsic spin–orbit interaction. The corresponding spin Hall and spin Nernst conductivities are compared with those obtained from effective low-energy $k \cdot p$ and reduced Hamiltonians, which are appropriate for states in the vicinity of the Fermi level of a neutral bilayer graphene. Both conductivities are determined within the linear response theory and Green function formalism. The influence of an external voltage between the two atomic sheets is also considered. The results reveal a transition from the topological spin Hall insulator phase at low voltages to conventional insulator phase at larger voltages.

(Some figures may appear in colour only in the online journal)

1. Introduction

Four decades ago Dyakonov and Perel showed that a system with strong spin–orbit interaction should reveal transverse spin current and spin accumulation in the presence of external electric field [1, 2]—even if the system is nonmagnetic. This effect, known now as the spin Hall effect (SHE) [3], has been studied extensively in the last few years [3–9], and is still of current interest—mainly because it offers a new possibility of spin manipulation with electric field only. The possibility of pure electrical manipulation of spin degrees of freedom is interesting not only for fundamental reasons, but also from the point of view of possible applications in future spintronics devices and information processing technologies [10–13].

The crucial interaction responsible for SHE, i.e. the spin–orbit coupling, may be either of intrinsic (internal) or extrinsic origin. The corresponding extrinsic SHE is associated with mechanisms of spin–orbit scattering on impurities and other defects (skew scattering and/or side jump), while the intrinsic SHE is a consequence of a nontrivial trajectory of charge carriers in the momentum space due to the spin–orbit contribution of a perfect crystal lattice to the corresponding band structure. The intrinsic SHE may be described in terms of the Berry phase formalism [14, 15] and therefore it is also referred to as the topological SHE.

It is well known that various spin effects, like for instance spin current and spin accumulation, may be generated not only by external electric field, but also due to a temperature gradient. Indeed, there is a great interest currently in spin related thermoelectric effects. One such phenomenon is the spin Seebeck effect, where longitudinal spin current and spin voltage are generated by a temperature gradient [16]. Of particular interest, however, are spin thermoelectric effects in systems with spin–orbit interaction, where a temperature gradient gives rise to transverse spin accumulation and/or spin currents. Thus, the temperature gradient in such systems may lead to anomalous (in the case of ferromagnetic systems) and spin Nernst effects [17–19], which correspond to the anomalous and spin Hall effects induced by electric field. The similarity between the spin Hall and spin Nernst effects in nonmagnetic systems with spin–orbit interaction is presented in figure 1, which clearly shows that the SHE is generated by external electric field, while the spin Nernst effect (SNE) is a similar effect generated by a temperature gradient instead of electric field (gradient of electrostatic potential).

In this paper we consider the topological contribution to the spin Hall and spin Nernst effects in a bilayer graphene.
Graphene is a two-dimensional crystal of carbon atoms. A monolayer graphene in a free standing form was obtained a few years ago and owing to its unusual and peculiar properties quickly became one of the most extensively studied materials [20–22]. After the pioneering paper by Kane and Mele [23], the spin Hall effect in a monolayer graphene was studied in many papers and in various physical situations [24–27]. Recently, bilayer graphene is being extensively studied as it is more appropriate for applications than a single-layer graphene. Moreover, it has been shown that spin–orbit coupling in a bilayer can be enhanced in comparison to that in a single-layer graphene [28]. This motivated us to consider topological contributions to the SHE and SNE in a bilayer graphene.

Both SHE and SNE in (nonmagnetic) graphene are generated by spin–orbit interaction. In general, one can distinguish two different forms of the spin–orbit interaction having the crystal lattice periodicity and contributing to the relevant band structure—internal and Rashba spin–orbit interactions. The latter interaction is due to a substrate and can be controlled by an external gate voltage. In this paper we consider the contributions to SHE and SNE due to the intrinsic spin–orbit interaction only. It is known that this interaction opens up an energy gap at the Dirac points. It was also shown that the energy gap can be tuned externally by applying a voltage bias between the layers [29, 30]. The gate voltage dependence of the spin Hall conductivity, leading to phase transition between the spin Hall insulator and classical insulator is also considered in this paper.

The description of transport properties of graphene is usually based on some effective Hamiltonians, which properly describe the electronic spectrum near the Fermi level of a neutral system. However, it is well known that the topological contribution to the spin Hall effect includes contributions from electronic states far below the Fermi level, and therefore a more accurate electronic spectrum is required to describe the effect properly. Accordingly, in this paper we calculate the spin Hall and spin Nernst conductivities for both cases the intrinsic spin–orbit interaction and the effect of a normal bias voltage are taken into account. In section 3 we calculate the spin Hall and spin Nernst conductivities for the effective $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian and compare them with those obtained from the tight binding Hamiltonian. In the former case we derive analytical formulas for the spin Hall and spin Nernst conductivities. We also discuss the role of normal bias (in the framework of the effective $\mathbf{k} \cdot \mathbf{p}$ model). Description based on a reduced low-energy effective Hamiltonian is presented in section 4. Summary and final conclusions are given in section 5.

2. Electronic spectrum of the bilayer graphene

A single-layer graphene is a monolayer of carbon atoms arranged in a two-dimensional honeycomb lattice which can be also considered as being composed of two nonequivalent triangular sublattices. In the absence of spin–orbit interaction, the Fermi surface of a neutral single-layer graphene consists of two nonequivalent K and K' points of the Brillouin zone, at which the valence and conduction bands touch each other. The corresponding electronic spectrum can be described by a tight binding Hamiltonian with nearest and next-nearest-neighbor hopping terms. The low-energy electron states near the points K and K' can be well approximated by a conical energy spectrum (linear dispersion relations). As a result, charge carriers in the vicinity of the points K and K' are described effectively by the relativistic Dirac equation [20, 21]. Intrinsic spin–orbit interaction then opens up an energy gap at the Dirac points [23]. The tight binding and effective $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians for a bilayer graphene are more complex, as described below.

2.1. Tight binding model

The bilayer graphene in the Bernal stacking (see e.g. [22]) is described by the following tight binding Hamiltonian:

$$\mathcal{H} = \int d^2 \mathbf{k} \psi^\dagger(\mathbf{k}) \begin{pmatrix} \mathbf{H} + V & \Gamma \\ \Gamma^\dagger & \mathbf{H} - V \end{pmatrix} \psi(\mathbf{k}),$$

where

$$\mathbf{H} = \begin{pmatrix} h_{00} S_z & h_{0s} S_0 \\ h_{s0} S_0 & -h_{00} S_z \end{pmatrix},$$

within the tight binding Hamiltonian and also in terms of an effective $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. The latter is sufficient for states in the vicinity of the Fermi level of a neutral graphene. In both cases the intrinsic spin–orbit interaction and the effect of a normal bias voltage are taken into account. In section 3 we calculate the spin Hall and spin Nernst conductivities for the effective $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian and compare them with those obtained from the tight binding Hamiltonian. In the former case we derive analytical formulas for the spin Hall and spin Nernst conductivities. We also discuss the role of normal bias (in the framework of the effective $\mathbf{k} \cdot \mathbf{p}$ model). Description based on a reduced low-energy effective Hamiltonian is presented in section 4. Summary and final conclusions are given in section 5.
The matrix elements $h_0$ and $h_{so}$ are defined as $h_0 = -i[t(e^{i2bk_y} + 2 \cos(\frac{i}{d}ak_x)e^{-i2bk_y})]$ and $h_{so} = -2t'\sin(ak_x) - 2\sin(ak_y)\cos(bk_y)$, where $t$ is the hopping integral between the nearest neighbors in the atomic sheets, $t'$ is the next-nearest-neighbor spin–orbit hopping amplitude, while $b = a\sqrt{3}/2$ with $a$ being the lattice parameter. Furthermore, $V$ is the voltage between the two atomic sheets of the bilayer (measured in energy units), $S_0$ denote the unit ($\alpha = 0$) and Pauli ($\alpha = x, y, z$) matrices in the spin space, while $\gamma_1$ describes coupling between the two atomic layers. We note that the spin–orbit hopping term originates from atomic spin–orbit interactions. Symmetry of graphene excludes spin–orbit coupling in the nearest-neighbor hopping term, but admits such a coupling in the next-nearest-neighbor term. A detailed description of the contributions from p and d orbitals to the spin–orbit interaction is presented in [28, 31, 32].

The corresponding energy eigenvalues for $V = 0$ have the following form:

$$E_{1,2} = ± \left[ h_0^2 + h_{so}^2 + V^2 + \frac{\gamma_1^2}{2} \right]^{1/2}. \quad (3)$$

$$E_{3,4} = ± \left[ h_0^2 + h_{so}^2 + V^2 + \frac{\gamma_1^2}{2} \right]^{1/2}. \quad (4)$$

This spectrum is shown in figure 2(a). States near the point K are shown by the solid lines in parts (b) and (c). The part (c) reveals a small energy gap created at the Dirac points by the spin–orbit interaction. Note, the chemical potential $\mu_0$ of a neutral graphene is assumed as zero of energy, $\mu_0 = 0$.

When $V \neq 0$, the inversion symmetry is broken (layers are no longer equivalent) and the degeneracy is lifted. The corresponding eigenvalues then acquire the form

$$E_{1,2} = ± \left[ h_0^2 + h_{so}^2 + V^2 + \frac{\gamma_1^2}{2} \right. \right. \nonumber
- \frac{1}{2}(\gamma_1^2 - 4Vh_{so})^2 + 4(\gamma_1^2 + 4V^2)h_{so}^2 \left]^{1/2}. \quad (5)$$

$$E_{3,4} = ± \left[ h_0^2 + h_{so}^2 + V^2 + \frac{\gamma_1^2}{2} \right. \nonumber
+ \frac{1}{2}(\gamma_1^2 - 4Vh_{so})^2 + 4(\gamma_1^2 + 4V^2)h_{so}^2 \left]^{1/2}. \quad (6)$$

The corresponding spectrum for the assumed value of $V/t = 0.01$ is indistinguishable from the spectrum shown in figure 2(a) for $V = 0$. The differences can be seen on a smaller energy scale, as in the parts (d) and (e) of figure 2. When comparing figures 2(b) and (d), one can notice a larger energy gap for $V/t = 0.01$. This is more clearly seen when comparing the parts (c) and (e). First, for the assumed value of V the gap is wider than for $V = 0$. Second, the top and bottom band edges become split and shifted away from the Dirac points. As will be described later, the applied voltage between the atomic sheets first closes the gap and then opens a new one with the width increasing with $V$.

2.2. Effective $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian

When only electronic states near the Fermi level (near the Dirac points) of a neutral graphene are relevant, one can
make use of some effective Hamiltonians to describe the corresponding electronic spectrum. Such a Hamiltonian can be derived using the \( \mathbf{k} \cdot \mathbf{p} \) approximation. As a result, the effective \( \mathbf{k} \cdot \mathbf{p} \) Hamiltonian for states near the K point of the bilayer graphene takes the form [33, 34]:

\[
H_K = T_0 \otimes H_K^0 + VT_x \otimes \sigma_0 \otimes S_0 - \frac{\gamma_1}{2} (T_x \otimes \sigma_x \otimes S_0 - T_y \otimes \sigma_y \otimes S_0),
\]

where \( H_K^0 = v(k_x \sigma_x + k_y \gamma_1) \otimes S_0 + \Delta_{so} \sigma_z \otimes S_2. \)

The first term on the right side of equation (10) corresponds to two decoupled atomic monolayers, each of them being described by the Kane Hamiltonian for a single-layer graphene, \( H_K^0 \). In turn, the second term takes into account the voltage between the layers, while the third term describes coupling between the monolayers, with \( T_0 \) denoting respectively the unit matrix \((\sigma = 0)\) and Pauli \((\sigma = x, y, z)\) matrices associated with the layer degree of freedom. Furthermore, \( \sigma_x (\sigma = 0, x, y, z) \) are the unit \((\sigma = 0)\) and Pauli \((\sigma = x, y, z)\) matrices in the pseudo-spin (sublattice) space. Relations between the parameters of the tight binding and Kane models are: \( v = \sqrt{3}a/2 = hv_F \) (\( v_F \) is the carrier velocity at the Fermi level) and \( \Delta_{so} = 3\sqrt{3}v_F \).

The eigenvalues of Hamiltonian (10) for \( v \neq 0 \) take the form

\[
E_{1,2} = \mp \left[ k^2v^2 + \frac{\gamma_1^2}{2} + \Delta_{so}^2 - \frac{\gamma_1}{2} \sqrt{4k^2v^2 + \gamma_1^2} \right]^{1/2},
\]

and

\[
E_{3,4} = \mp \left[ k^2v^2 + \frac{\gamma_1^2}{2} + \Delta_{so}^2 + \frac{\gamma_1}{2} \sqrt{4k^2v^2 + \gamma_1^2} \right]^{1/2}.
\]

The electronic spectrum near the point K, described by the above formula, is shown in figures 2(b) and (c), where it is compared with the spectrum obtained from the full tight binding Hamiltonian. Close to the K point, spectra from both models coincide very well.

When \( v \neq 0 \), one finds

\[
E_{1,2} = \mp \left[ k^2v^2 + \Delta_{so}^2 + v^2 + \frac{\gamma_1^2}{2} - \frac{1}{2}(\gamma_1^2 - 4\Delta_{so}^2) \right]^{1/2},
\]

\[
E_{3,4} = \mp \left[ k^2v^2 + \Delta_{so}^2 + v^2 + \frac{\gamma_1^2}{2} + \frac{1}{2}(\gamma_1^2 + 4\Delta_{so}^2) \right]^{1/2},
\]

The above spectrum is shown in figures 2(d) and (e), where it is compared with the corresponding spectrum obtained in the tight binding model. As before, spectra from the tight binding and effective \( \mathbf{k} \cdot \mathbf{p} \) models coincide near the K point. Note, the band splitting due to \( V \) is well resolved (for the assumed value of \( V \)) only in part (e).

Separation of the bands \( E_3 \) and \( E_4 \) in the effective model described above, as well as in the tight binding model, is much larger than the separation of the bands \( E_1 \) and \( E_2 \), see figure 2. Therefore, when the electronic states close to the band edges are relevant and sufficient to describe transport properties (e.g., when the Fermi level is in the gap), one may restrict considerations to the bands \( E_1 \) and \( E_2 \). This leads to a further simplification of the effective Hamiltonian, as described in more detail in section 4.

3. Spin Hall and spin Nernst effects

Spin Hall and spin Nernst effects correspond to transversal spin currents induced by electric field and temperature gradient, respectively. By analogy to the usual Hall and Nernst effects one may write the density of spin current due to electric field \( \mathbf{E} \) and temperature gradient \( \nabla T \) as

\[
\mathbf{J}^\nu = \sum_j [\sigma_{ij}^\nu E_j + \alpha_{ij}^\nu (-\partial_j T)],
\]

where \( \sigma_{ij}^\nu \) (for \( i, j = x, y \)) is the spin Hall conductivity, with \( \alpha_{ij}^\nu \) being the \( n \)th component (\( n = x, y, z \)) of electron spin, while \( \alpha_{ij}^\nu \) denotes the spin Nernst conductivity. In practice, the electric field and temperature gradient are due to a finite voltage and finite temperature difference between the two reservoirs attached to the sample, respectively. In turn, to measure the spin current one can make use of the inverse spin Hall effect and the sample geometry as proposed in [3]. The two conductivities are not independent and obey some general relations. Our objective is to find first the zero-temperature spin Hall conductivity, and then to calculate the low-temperature thermoelectric spin Hall conductivity from these relations, as described below.

The quantum-mechanical operator of spin current density may be defined as

\[
\mathbf{J}^\nu = \frac{1}{2} [\mathbf{v}, s_n i],
\]

where \([A, B]_+ = AB + BA\) denotes the anticommutator of any two operators \( A \) and \( B \), while \( v_i = (1/\hbar)(\partial H/\partial k_i) \) is the velocity operator \((i = x, y, z)\). The latter operator can be easily found from the corresponding Hamiltonian (equations (1) and (10)). In the linear response theory, the frequency-dependent spin Hall conductivity is then given by the formula [27, 35–38],

\[
\sigma_{ij}^\nu(\omega) = \frac{e}{2\omega} \text{Tr} \int \frac{d\mathbf{k}}{2\pi} \frac{d\epsilon}{2\pi(2\pi)^2} [v_\nu^x(s_2)] G_\mathbf{k}(\epsilon + \omega)v_\gamma^y G_\mathbf{k}(\epsilon),
\]

where 4
where $G_k(\varepsilon)$ is the Green function corresponding to the appropriate Hamiltonian of the system. The Green functions, and therefore also the conductivity $\sigma_{xy}^s(\omega)$ depend on the chemical potential $\mu$, which however is not indicated explicitly for brevity reasons. This formula gives exactly the same result as that based on the Berry phase calculations [14] in momentum space. In the following we analyze in detail $dc/\omega$ (as well as spin Nernst) conductivity; $\sigma_{xy}^s(\omega \rightarrow 0) \equiv \sigma_{xy}^s$.

It has been shown that the Berry phase leads to an additional term in the general expression for the orbital magnetization [39]. This correction gives rise to some contributions to the charge transport, and will be used to write a relationship between intrinsic spin Nernst conductivity and intrinsic zero-temperature spin Hall conductivity, which in the low-temperature regime takes the form [40]

$$\sigma_{xy}^s = \frac{\pi^2 k_B^2}{3e^2} T \frac{d\sigma_{xy}^s}{d\mu},$$

(21)

where $T$ stands for temperature and $k_B$ denotes the Boltzmann constant. The latter equation is the spin analog of the Mott relation for charge transport, and will be used to calculate the low-temperature spin Nernst conductivity from the zero-temperature spin Hall conductivity. The Mott’s formula (21) holds when $\sigma_{xy}^s$ varies rather slowly with the Fermi level. Thus, in this case one may expect this formula may be violated when the Fermi level approaches the band edges [41].

Thus, we need to calculate the spin Hall conductivity first. The relevant derivation depends on the model applied to describe the corresponding electronic spectrum. Below we present derivation of the spin Hall and spin Nernst conductivities for the effective $k \cdot p$ Hamiltonian, where analytical results are available. These results will be compared with those obtained numerically for the tight binding model.

3.1. The limit of $V = 0$

Assume first the limit of $V = 0$. To find the spin Hall conductivity we start from equation (20) and write it in the form

$$\sigma_{xy}^s(\omega) = \frac{e}{2\omega} \int \frac{dc}{2\pi} \int \frac{d^2k}{(2\pi)^2} D(\varepsilon + \omega, \varepsilon)$$

where

$$\times \frac{4}{n+1}[\varepsilon - E_n + \omega + \mu + i\delta \text{sgn}(\varepsilon)]^{-2}$$

$$\times \frac{4}{n+1}[\varepsilon - E_m + \mu + i\delta \text{sgn}(\varepsilon)]^{-2}.$$ (22)

Here $D(\varepsilon + \omega, \varepsilon)$ is defined as

$$D(\varepsilon + \omega, \varepsilon) = \text{Tr}[[v_x, s_+], g_k(\varepsilon + \omega) v_y g_k(\varepsilon)],$$

(23)

where $g_k(\varepsilon)$ denotes the nominator of the corresponding Green function $G_k(\varepsilon)$. For brevity reasons, the $k$-dependence of $D(\varepsilon + \omega, \varepsilon)$ (as well as of $\chi(\varepsilon)$ and $F(\varepsilon)$ below) has not been indicated explicitly.

Taking the first two terms of the expansion of $D(\varepsilon + \omega, \varepsilon)$ with respect to $\omega_0$, one finds

$$D(\varepsilon + \omega, \varepsilon) \approx i\omega \chi(\varepsilon),$$

(24)

with

$$\chi(\varepsilon) = 8\pi^2 \Delta_{so} [v^2 k^2 + 2(\Delta^2 - (\varepsilon - \mu)^2)]$$

$$+ (\Delta_{so}^2 - (\varepsilon + \mu)^2)(\gamma_1^2 + \Delta_{so}^2 - (\varepsilon + \mu)^2)^2$$

$$\times (\Delta_{so}^2 - (\varepsilon + \mu)^2)(\gamma_2^2 + \Delta_{so}^2 - (\varepsilon + \mu)^2)$$

$$+ v^2 k^2 [v^2 k^2 + 2(\gamma_1^2 + \Delta_{so}^2 - (\varepsilon + \mu)^2)].$$ (25)

Thus, in the limit of $\omega \rightarrow 0$ one finds the following expression for the spin Hall conductivity

$$\sigma_{xy}^s = \frac{i e}{2} \int \frac{dc}{2\pi} \int \frac{d^2k}{(2\pi)^2} F(\varepsilon),$$

(26)

where

$$F(\varepsilon) = \frac{\chi(\varepsilon)}{\prod_{\gamma=1}^{n}[\varepsilon - E_n + \mu \pm i\delta \text{sgn}(\varepsilon)]^4}.$$ (27)

Integrating now over $\varepsilon$ one finds

$$\int d\varepsilon F(\varepsilon) = 2\pi i \sum_n R_n f(E_n),$$

(28)

where $R_n$ ($n = 1 \rightarrow 4$) are the residua associated with the corresponding self-energies (electron bands), and $f(E)$ is the Fermi distribution function (here for zero temperature). These residua are equal:

$$R_{1,2} = \pm \frac{4\sqrt{2}\pi^2 \Delta_{so}[2v^2 k^2(\gamma_1 + \xi) + \gamma_1(\gamma_1^2 - \gamma_1 \xi + 2\Delta_{so}^2)]}{\xi^3(2v^2 k^2 + \gamma_1^2 - \gamma_1 \xi + 2\Delta_{so}^2)^{3/2}}$$

(29)

and

$$R_{3,4} = \pm \frac{8\sqrt{2}\pi^2 \Delta_{so}}{\xi^3(2v^2 k^2 + \gamma_1^2 + \gamma_1 \xi + 2\Delta_{so}^2)^{3/2}}$$

(30)

with

$$L = -v^2 k^2(3\gamma_1^2 + \gamma_1 \xi + 4\gamma_1 \Delta_{so} - 2\xi \Delta_{so}^2 + 2v^2 k^2(\gamma_1 + \xi)$$

$$- \gamma_1(\gamma_1^2 + \gamma_1 \xi + 2\gamma_1 \Delta_{so} + 2\gamma_1 \xi \Delta_{so} + 2\Delta_{so}^2),$$

(31)

where $\xi = \sqrt{4\pi^2 k^2 + \gamma_1^2}$. Thus, the conductivity may be written in the form

$$\sigma_{xy}^s = -\frac{e}{4\pi} \sum_n \int k R_n f(E_n) dk.$$ (32)

Taking into account the indefinite integrals

$$\int k R_1 dk = -\frac{\sqrt{2}(\gamma_1 + \xi) \Delta_{so}}{\xi(2v^2 k^2 + \gamma_1^2 + \gamma_1 \xi + 2\Delta_{so}^2)^{1/2}},$$

(33)

$$\int k R_3 dk = \frac{\sqrt{2}(\gamma_1 - \xi) \Delta_{so}}{\xi(2v^2 k^2 + \gamma_1^2 + \gamma_1 \xi + 2\Delta_{so}^2)^{1/2}},$$

(34)
and then assuming the appropriate limits of the integration, one finds the final expressions for the spin Hall conductivity as presented below.

When the chemical level is inside the gap, \(|\mu| < \Delta_{so}\), the spin Hall conductivity is equal to

$$\sigma_{xy}^{s} = -\frac{2\sigma}{4\pi}.$$  \hspace{1cm} (35)

When \(\Delta_{so} < |\mu| < \sqrt{\gamma_{1}^{2} + \Delta_{so}^{2}}\),

$$\sigma_{xy}^{s} = -\frac{2(\gamma_{1} + \sqrt{\mu^{2} - \Delta_{so}^{2}}) \Delta_{so} e}{2\sqrt{\mu^{2} - \Delta_{so}^{2}} + \gamma_{1} |\mu|}.$$

$$\frac{4\pi}{\mu^{2} - \Delta_{so}^{2} + \gamma_{1} |\mu|}.$$ \hspace{1cm} (36)

while for \(|\mu| > \sqrt{\gamma_{1}^{2} + \Delta_{so}^{2}}\) one finds

$$\sigma_{xy}^{s} = -\frac{2(\mu^{2} - \Delta_{so}^{2}) - \gamma_{1}^{2} + 4\Delta_{so} e}{4(\mu^{2} - \Delta_{so}^{2}) - \gamma_{1}^{2} |\mu|}.$$

$$\frac{4\pi}{\mu^{2} - \Delta_{so}^{2} + \gamma_{1} |\mu|}.$$ \hspace{1cm} (37)

The spin Hall conductivity inside the gap is now twice as large as that in the case of a single-layer graphene. The general behavior of the conductivity with position of the Fermi level, shown in figure 3 by the solid dark (solid red) line, is qualitatively similar to that for a single-layer graphene, i.e. outside the gap the spin Hall conductivity tends to zero with increasing \(|\mu|\), while it remains constant and quantized inside the gap. This behavior is reasonable as the spin Hall conductivity is due to spin–orbit coupling, which may follow from the inapplicability of Mott’s formula (21) at \(\mu = 0\) and other parameters as in figure 2.

Figure 3. Spin Hall and spin Nernst conductivities of a bilayer graphene for \(V = 0\) and other parameters as in figure 2. Contributions from both K and K’ points are included. The solid lines correspond to the results obtained from the effective Hamiltonian (10), while the dots correspond to the tight binding model. The blue line. Similarly to a single-layer graphene \([18]\), the spin Nernst conductivity vanishes for the Fermi level inside the gap, when the system is in the insulating phase, and becomes nonzero for the Fermi level inside the valence or conduction bands, when the temperature gradient generates a longitudinal charge current. Note, the spin Nernst conductivity becomes divergent as \(\mu\) approaches the edges of the energy gap. This may follow from the inapplicability of Mott’s formula (21) at the band edges.

Conductivity in the tight binding model can be obtained in a similar way, although the corresponding formulas are cumbersome and will not be presented here. Instead of this we present some numerical results, which in figure 3 are shown by the dots. Note, the spin Hall as well as spin Nernst conductivities in the effective model coincide very well with the results obtained from the tight binding model.

3.2. The case of \(V \neq 0\)

Let us consider now the case of \(V \neq 0\). The procedure presented above for the effective model with \(V = 0\) can be easily extended to a nonzero vertical bias, \(V \neq 0\). The difference is that now the degeneracy of the bands is lifted and we have eight different bands, \(n = 1–8\), which have to be taken into account. Thus, instead of equation (27) we have now

$$\mathcal{F}(\varepsilon) = \frac{\chi(\varepsilon)}{\prod_{n=1}^{8}[\varepsilon - E_{n} + i\delta \text{sgn}(\varepsilon)]^2}.$$ \hspace{1cm} (40)

with adequate \(\chi(\varepsilon)\). Following the procedure described above for \(V = 0\), one can derive the corresponding analytical formulas. These formulas, however, will not be presented here as they are rather cumbersome, so we present only numerical results. Moreover, since the results in the tight binding model coincide with those obtained with the effective Hamiltonian, as shown above, we restrict the analysis below to the effective Hamiltonian.
Figure 4. Zero-temperature spin Hall conductivity as a function of the vertical voltage $V$ and position of the Fermi level for the effective model described by the parameters given in figure 2. Contributions from both Dirac points are included. The vertical dashed line corresponds to $V$, where transition from the spin Hall insulator phase to the conventional insulator one takes place.

Figure 5. Zero-temperature spin Hall conductivity as a function of vertical bias voltage $V$ for indicated values of the Fermi energy. The curves correspond to cross-sections of figure 4 along constant $\mu$. The other parameters are as in figure 4.

In figure 4 we show the spin Hall conductivity as a function of the Fermi level $\mu$ and vertical bias $V$. For $V = 0$ we recover the quantized conductivity in the gap. As $V$ increases, however, the range of quantized spin Hall conductivity shrinks and at $V = \Delta_{so}$ (indicated by the dashed line in figure 4) there is a transition (at $\mu = 0$) from $\sigma_{xy}^{z} = -4(e/4\pi)$ to 0. This behavior is explicitly shown in figure 5, where several cross-sections of figure 4 along constant values of $\mu$ are presented. The above transition is clearly evident for the curve corresponding to $\mu = 0$.

The transition from topological insulating phase at small voltages to the normal insulating behavior at large voltages is also clearly visible in figure 6, which presents some cross-sections of figure 4 along constant values of $V$. This figure shows how the range of the quantized value of $\sigma_{xy}^{z}$ changes with increasing $V$. As $V$ increases starting from $V = 0$, the width of the range where $\sigma_{xy}^{z}$ is quantized shrinks and turns to zero at the critical value of $V$. The spin Hall conductivity $\sigma_{xy}^{z}$ at $\mu = 0$ changes then from $\sigma_{xy}^{z} = -4(e/4\pi)$ at voltages smaller than the critical one to $\sigma_{xy}^{z} = 0$ at higher voltages. This clearly reveals a transition from the topological insulating phase to the normal insulating behavior (more information on the topological insulating phases in graphene can be found e.g. in [42]). From figures 4 to 6 one can conclude that the gap diminishes with increasing $V$, becomes totally suppressed at the critical value of $V$, and then becomes open again at larger voltages. Indeed, this is the case as shown in figure 7, where the spectrum near the gap is plotted for several values of $V$. This figure clearly shows that the gap becomes closed at the critical value of $V$, and then is open again at larger voltages. The spin Hall conductivity in the gap above the critical voltage is, however, suppressed.

We note that in a recent paper Qiao et al. [43] considered topological phase transitions in a bilayer graphene with Rashba spin–orbit interaction, induced by a voltage applied between the two atomic monolayers. In our case we have found topological phase transition induced by gate voltage in a bilayer graphene with intrinsic spin–orbit coupling.

The phase transition from the topological spin Hall insulating phase to the conventional insulator becomes revealed in the spin Nernst conductivity, too. This is presented in figure 8, where the low-temperature spin Nernst conductivity is shown as a function of the chemical potential for the same values of $V$ as in figure 6. The range of zero spin
Nernst conductivity decreases with increasing $V$, goes to zero at the critical value of $V (V = \Delta_{so})$, and then becomes nonzero again for larger values of $V$. 

4. Reduced low-energy Hamiltonian

As we have already mentioned above, separation of the bands $E_3$ and $E_4$ (or $E_{3,\gamma}$ and $E_{4,\delta}$) is much larger than separation of the bands $E_1$ and $E_2$ (or $E_{1,\gamma'}$ and $E_{2,\gamma'}$). The latter determines the energy gap induced by the spin–orbit coupling (see figure 2). When only the electron states near the Fermi level are relevant and the Fermi level is in the gap or close to it, one may further reduce the effective Hamiltonian to include explicitly the bands $E_{1,\gamma'}$ and $E_{2,\gamma'}$, and the other bands only via effective parameters of the corresponding reduced effective model. The relevant reduced low-energy effective Hamiltonian takes the form [34]:

$$H_{\gamma} = \begin{pmatrix}
\Delta_{so} + V & 0 & -\frac{h^2 k^2}{2m} & 0 \\
0 & -\Delta_{so} + V & 0 & \frac{h^2 k^2}{2m} \\
-\frac{h^2 k^2}{2m} & 0 & -\Delta_{so} - V & 0 \\
0 & -\frac{h^2 k^2}{2m} & 0 & \Delta_{so} - V
\end{pmatrix}, \quad (41)$$

where $k_\gamma = k_x \pm i k_y$ and $m = \gamma_1/2v_F$ is the effective electron mass. In the following we consider some special cases.

4.1. The case of $V = 0$

The corresponding eigenvalues of the Hamiltonian (41) are then equal to

$$E_{1,2} = \pm \left[ \Delta_{so}^2 + \left( \frac{h^2 k^2}{2m} \right)^2 \right]^{1/2}. \quad (42)$$

Using the notation introduced in the preceding section we find

$$\sigma_{xy}^{e_\gamma} = -\frac{2}{|\mu|} \frac{e}{4\pi}$$

for $|\mu| > \Delta_{so}$, and

$$\sigma_{xy}^{e_\gamma} = -\frac{2}{|\mu|} \frac{e}{4\pi}$$

when the chemical level is inside the gap, $|\mu| < \Delta_{so}$.

The corresponding low-temperature spin Nernst conductivity is then given as follows. For $|\mu| > \Delta_{so}$ one finds

$$\alpha_{xy}^{e_\gamma} = \frac{\pi}{6} \frac{e^2}{h} \frac{\Delta_{so}}{\mu^2} T,$$

while for $\mu$ inside the gap $\alpha_{xy}^{e_\gamma} = 0$. 

4.2. The case of $V > \Delta_{so}$

The low-temperature spin Nernst conductivity as a function of the chemical potential for indicated values of $V$, calculated for the same parameters as in figure 6.
The above results for both spin Hall and spin Nernst conductivities are shown by the dots in figure 9, where they are compared with the corresponding results obtained from the effective Hamiltonian (10) (solid lines). There is a nice agreement between the results. We note that the divergency of the spin Nernst conductivity when the Fermi level approaches the band edges, observed in the tight binding and effective Hamiltonian model, is not reproduced in the reduced low-energy Hamiltonian.

4.2. The case of \( V \neq 0 \)

When \( V \neq 0 \) the eigenvalues of the Hamiltonian (41) take the form:

\[
E_{1,2} = \pi \left[ (V + \Delta_{so})^2 + \left( \frac{\hbar^2 k^2}{2m} \right)^2 \right]^{1/2},
\]

\[
E_{1',2'} = \pi \left[ (V - \Delta_{so})^2 + \left( \frac{\hbar^2 k^2}{2m} \right)^2 \right]^{1/2}.
\]

The nonzero \( V \) leads to splitting of the electron bands, as already discussed above.

The spin Hall conductivity can be obtained analogously as in the case of \( V = 0 \). When \( |\mu| > (V + \Delta_{so}) \), one then finds

\[
\sigma_{xy}^{\alpha} = -\frac{e}{4\pi} \frac{1}{|\mu|} \Delta_{so},
\]

When \( |V - \Delta_{so}| < |\mu| < (V + \Delta_{so}) \),

\[
\sigma_{xy}^{\alpha} = -\frac{e}{4\pi} \left( 1 - \frac{V - \Delta_{so}}{|\mu|} \right).
\]

Finally, when \( \mu \) is inside the gap

\[
\sigma_{xy}^{\alpha} = 0 \quad \text{for} \ V > \Delta_{so}.
\]
obtained results, however, will be modified when both Coulomb interaction and scattering by structural defects are included. This, however, requires additional considerations, which will be described and presented in a future paper.

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