Intrinsic Spin Hall and Spin Nernst Effects in Single-Layer Graphene: Tight-Binding vs. Effective Model

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We calculate topological contributions to the spin Hall and spin Nernst effects due to intrinsic spin–orbit interaction in a single-layer graphene. To describe electronic spectrum of the graphene we have assumed the $\boldsymbol{k} \cdot \boldsymbol{p}$ model as well as the full tight-binding Hamiltonian. The corresponding contributions to the spin Hall and spin Nernst effects have been determined using the linear response theory and Green function formalism.

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1. Introduction

Spin Hall effect (SHE) [1–3] is currently extensively studied — mainly because it offers a new possibility of spin manipulation using electric field only (for review see e.g. [4]). The crucial interaction leading to SHE is the spin–orbit coupling, either of extrinsic or intrinsic (internal) origin. The corresponding extrinsic SHE is associated with spin–orbit scattering mechanisms 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 spin–orbit contribution of a perfect crystal to the corresponding band structure. The intrinsic SHE may be described in terms of the Berry phase [5, 6] and therefore it is also referred to as the topological SHE. In turn, the spin Nernst effect (SNE) is very similar to SHE, except that the spin current is driven by temperature gradient.

In this paper we consider the topological contributions to the spin Hall and spin Nernst effects in a single-layer graphene. Graphene is a two-dimensional honeycomb lattice of carbon atoms, with two nonequivalent 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 electron states near the K and K' points can be approximated by a conical energy spectrum. As a result, charge carriers in the vicinity of the points K and K' are described by the relativistic Dirac equation [7, 8]. As shown by Kane and Mele [9], intrinsic spin–orbit interaction opens an energy gap at the Dirac points, and also leads to a quantized and universal value of the spin Hall conductivity when the Fermi level is inside the gap. However, when the Rashba spin–orbit interaction is stronger than the intrinsic one, the gap becomes closed. Here we consider a free-standing graphene sheet, where the Rashba interaction is absent.

Since all electron states below the Fermi level can contribute to the intrinsic SHE and SNE, one may expect that exact electronic band structure is important for the appropriate theoretical description of the effects. There-fore, we examine and compare intrinsic SHE and SNE in the tight-binding model and in the effective ($\boldsymbol{k} \cdot \boldsymbol{p}$) model. We show that there is perfect agreement between the spin Hall and spin Nernst conductivities obtained in both models of electronic structure. In Sect. 2 we introduce the tight-binding Hamiltonian for graphene and also effective $\boldsymbol{k} \cdot \boldsymbol{p}$ Hamiltonian for energy states near the Dirac points. The general formula for spin Hall conductivity is derived in Sect. 3. The analytical and numerical results for spin Hall and spin Nernst conductivities are presented and discussed in Sect. 4, while final conclusions are given in Sect. 5.

2. Hamiltonian of a single-layer graphene

Tight-binding Hamiltonian with the hopping term between nearest neighbors and also between next nearest neighbors appropriately describes the band structure of graphene. This Hamiltonian may be written in the pseudospin (sublattice) and spin spaces as [10, 11]:

$$\mathcal{H}_{\mathrm{G}} = -\int \mathrm{d}^2 \boldsymbol{k}\, \psi(\boldsymbol{k})^\dagger H \psi(\boldsymbol{k}) \tag{1}$$

with

$$H = \begin{pmatrix} h_{\mathrm{so}} S_z & h_0 S_0 \\ h_0^* S_0 & -h_{\mathrm{so}} S_z \end{pmatrix}, \tag{2}$$

where $h_0 = t[\mathrm{e}^{\mathrm{i}2bk_y/3} + 2\cos(ak_x/2)\,\mathrm{e}^{-\mathrm{i}bk_y/3}]$, $h_{\mathrm{so}} = 2t'[\sin(ak_x) - 2\sin(ak_x/2)\cos(bk_y)]$, and $b = a\sqrt{3}/2$. Here, t (≈ 2.8 eV) and t' are the hopping parameters between nearest and next nearest neighbors, respectively, while a is lattice constant (≈ 2.4 Å). Apart from this, S_z is the z component of the spin Pauli matrices, while S_0 is a unit matrix in the spin space. The eigenvalues of this Hamiltonian are

$$E_{1,2} = \mp\sqrt{h_0^2 + h_{\mathrm{so}}^2}. \tag{3}$$

Using the $\boldsymbol{k} \cdot \boldsymbol{p}$ approximation one can derive the well known effective Hamiltonian (known as the Kane Hamiltonian) for the states near the K and K' points of the Brillouin zone [9, 12]. This Hamiltonian for the K point has the form [9]:

$$H_K = v(k_x\sigma_x + k_y\sigma_y) \otimes S_0 + \Delta_{so}\sigma_z \otimes S_z, \qquad (4)$$

where $v = \sqrt{3}ta/2 = \hbar v_F$ (v_F is the carrier velocity at the Fermi level), while $\Delta_{so} = 3\sqrt{3}t'$ is the parameter of spin–orbit coupling. Furthermore, σ_i ($i = x, y, z$) are the Pauli matrices associated with the pseudospin (sublattice) degree of freedom. The eigenvalues of Hamiltonian (4) are

$$E_{1,2} = \mp\sqrt{\Delta_{so}^2 + v^2 k^2}. \qquad (5)$$

In Fig. 1 we show the electronic spectrum of the tight binding as well as effective Hamiltonians. Since the intrinsic spin–orbit coupling does not break the inversion symmetry of the graphene lattice, the spectrum is spin degenerate.
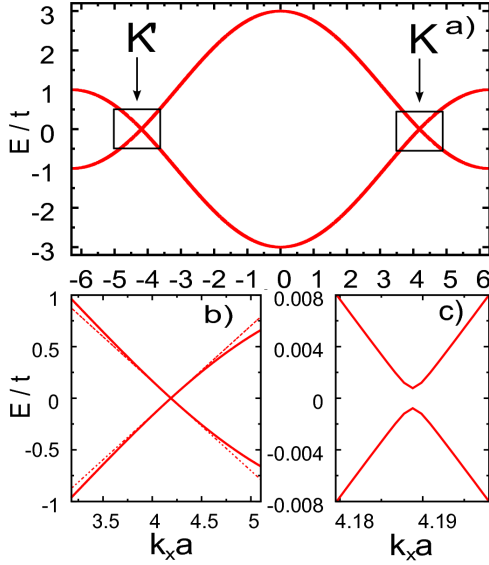

Fig. 1. (a) Electronic spectrum of graphene in the tight-binding model (for $k_y = 0$ and $t'/t = 0.00015$). (b) Part of the spectrum near the K point (the spectrum in the $\mathbf{k} \cdot \mathbf{p}$ effective Hamiltonian is also shown by the dotted lines). (c) Electronic spectrum in the very close vicinity of the K point, where the gap due to spin–orbit coupling is well resolved (now the spectra in both models are indistinguishable).

3. Spin Hall conductivity

Spin Hall and spin Nernst effects consist in transversal spin currents induced by electric field $\mathbf{E}$ and temperature gradient ∇T, respectively. Density of spin current can be thus written as

$$J_i^{s_n} = \sum_j \left[\sigma_{ij}^{s_n} E_j + \alpha_{ij}^{s_n}(-\partial_j T)\right], \qquad (6)$$

where $\sigma_{ij}^{s_n}$ (for $i, j = x, y$) is the spin conductivity with $s_n = (\hbar/2)\sigma_n$ being the n-th component ($n = x, y, z$) of electron spin, while $\alpha_{ij}^{s_n}$ denotes the thermoelectric spin Nernst conductivity.

The quantum-mechanical operator of spin current density may be defined as $\mathbf{J}^{s_n} = [\mathbf{v}, s_n]_+/2$, where $v_i = (1/\hbar)(\partial H/\partial k_i)$ is the velocity operator ($i = x, y$). In the

linear response theory, the frequency-dependent spin Hall conductivity is then given by the formula [13],

$$\sigma_{xy}^{s_z}(\omega) = \frac{e\hbar}{2\omega}\text{Tr} \int \frac{d\varepsilon}{2\pi}\frac{d^2\mathbf{k}}{(2\pi)^2}[v_x, s_z]_+$$
$$\times G_{\mathbf{k}}(\varepsilon + \omega)v_y G_{\mathbf{k}}(\varepsilon), \qquad (7)$$

where $G_{\mathbf{k}}(\varepsilon)$ is the Green function corresponding to the appropriate Hamiltonian of the system. When we restrict considerations to the topological contribution to the spin Hall current in the dc limit, this formula gives exactly the same result as that based on the calculation of the Berry phase [5] in the momentum space.

Thus, to find the spin Hall conductivity we start from Eq. (7) and calculate the trace

$$D(\varepsilon + \omega, \varepsilon) = \text{Tr}\{[v_x, s_z]_+ g_{\mathbf{k}}(\varepsilon + \omega)v_y g_{\mathbf{k}}(\varepsilon)\}, \qquad (8)$$

where $g_{\mathbf{k}}(\varepsilon)$ denotes the nominator of the Green function $G_{\mathbf{k}}(\varepsilon)$. Taking the first two terms of the expansion of D with respect to ω, one can write $D(\varepsilon + \omega, \varepsilon)$ as $D(\varepsilon + \omega, \varepsilon) \simeq i\omega\chi(\varepsilon)$. Then, in the limit of $\omega \to 0$ Eq. (7) gives

$$\sigma_{xy}^{s_z} = i\frac{e}{2}\int \frac{d\varepsilon}{2\pi}\int \frac{d^2\mathbf{k}}{(2\pi)^2}\mathcal{F}(\varepsilon), \qquad (9)$$

where

$$\mathcal{F}(\varepsilon) = \frac{\chi(\varepsilon)}{\prod_{n=1}^2(\varepsilon - E_n + \mu + i\delta\,\text{sgn}\,\varepsilon)^2}. \qquad (10)$$

Integrating $\mathcal{F}(\varepsilon)$ over energy leads to

$$\int d\varepsilon\mathcal{F}(\varepsilon) = 2\pi i\sum_n R_n f(E_n), \qquad (11)$$

where R_n ($n = 1$–2) are the residua associated with the corresponding electron bands, and $f(E)$ is the Fermi distribution function. Finally, the spin Hall conductivity can be written as

$$\sigma_{xy}^{s_z} = -\frac{e}{2}\sum_n \int \frac{d^2\mathbf{k}}{(2\pi)^2}R_n f(E_n). \qquad (12)$$

It has been shown that the intrinsic spin Nernst conductivity is related to the zero-temperature intrinsic spin Hall conductivity [14–16]. In the low temperature regime this relationship takes the form [16]

$$\alpha_{xy}^{s_z} = \frac{\pi^2 k_B^2}{3e} T\frac{d\sigma_{xy}^{s_z}}{d\varepsilon}\bigg|_{\varepsilon=\mu}, \qquad (13)$$

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 spin Nernst conductivity from the zero-temperature spin Hall conductivity. The derivative in Eq. (13) is taken at the Fermi level μ which can be tuned by an external gate voltage.

4. Results

Let us consider first the effective model, as it allows to find analytical formula for the spin Hall and spin Nernst conductivities. In the Kane Hamiltonian we find the well known solution (see [9, 13, 17])

$$\sigma_{xy}^{s_z} = -\frac{e}{4\pi}\frac{\Delta_{\mathrm{so}}}{|\mu|} \quad \text{for} \quad |\mu| > \Delta_{\mathrm{so}} \tag{14}$$

and

$$\sigma_{xy}^{s_z} = -\frac{e}{4\pi} \quad \text{for} \quad |\mu| \le \Delta_{\mathrm{so}}. \tag{15}$$

Taking now into account Eq. (13) and the above formula for zero-temperature spin Hall conductivity, one finds the low-temperature spin Nernst conductivity in the form

$$\alpha_{xy}^{s_z} = -\pi\Delta_{\mathrm{so}}k_{\mathrm{B}}^2 T/12\mu^2 \quad \text{for} \quad \mu < -\Delta_{\mathrm{so}}, \tag{16}$$

$$\alpha_{xy}^{s_z} = 0 \quad \text{when} \quad -\Delta_{\mathrm{so}} < \mu < \Delta_{\mathrm{so}}, \tag{17}$$

$$\alpha_{xy}^{s_z} = \pi\Delta_{\mathrm{so}}k_{\mathrm{B}}^2 T/12\mu^2 \quad \text{for} \quad \mu > \Delta_{\mathrm{so}}. \tag{18}$$

For the tight-binding model, in turn, the integration over k was done numerically. Results for spin Hall and spin Nernst conductivities, obtained from both models, are shown in Fig. 2. There is perfect agreement between the results obtained with the effective and full tight binding Hamiltonians. The spin Hall conductivity takes a quantized value inside the energy gap. The spin Nernst conductivity is nonzero only when the temperature gradient is associated with a charge current flowing through the system, i.e., the conductivity disappears when the chemical level is inside the energy gap open by the spin–orbit interaction. For μ outside the gap, the temperature gradient generates a longitudinal charge current, and the spin–orbit interaction leads then to a nonzero transverse spin current.
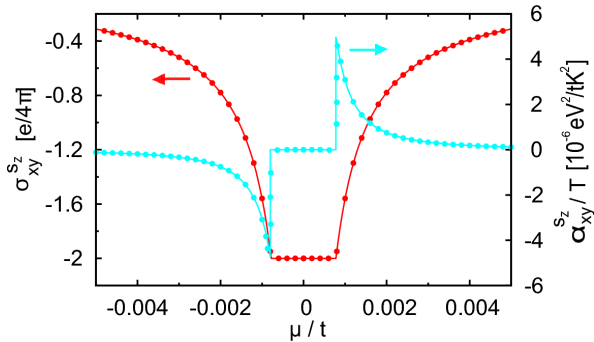

Fig. 2. Spin Hall (black/red) and spin Nernst (grey/blue) conductivity as a function of the Fermi level position. The results obtained in tight-binding model (dots) are in perfect agreement with those obtained with the effective Hamiltonian (solid lines). The parameters are taken as in Fig. 1.

5. Summary

We have calculated the spin Hall and spin Nernst conductivities in a single-layer graphene. To describe the relevant electronic spectrum we have assumed simplified effective Hamiltonian corresponding to states close to the Dirac points as well as the full tight-binding Hamiltonian. Both spin Hall and spin Nernst conductivities obtained in both models almost coincide, which is due to a small value of the intrinsic spin–orbit coupling in graphene. Thus, to describe intrinsic SHE and SNE in single-layer graphene one may consider the effective Hamiltonian.

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