Anomalous, spin, and valley Hall effects in graphene deposited on ferromagnetic substrates

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Keywords: graphene, hybrid systems, spin currents, valleytronics, spintronics

Abstract
Spin, anomalous, and valley Hall effects in graphene-based hybrid structures are studied theoretically within the Green function formalism and linear response theory. Two different types of hybrid systems are considered in detail: (i) graphene/boron nitride/ferromagnetic metal (cobalt or nickel), and (ii) graphene/magnetic insulator (YIG). The main interest is focused on the proximity-induced exchange interaction between graphene and magnetic substrate and on the proximity-enhanced spin–orbit coupling. The proximity effects are shown to have a significant influence on the electronic and spin transport properties of graphene. To find the spin, anomalous and valley Hall conductivities we employ certain effective Hamiltonians which have been proposed recently for the hybrid systems under considerations. Both anomalous and valley Hall conductivities are shown to have universal values when the Fermi level is inside the energy gap in the electronic spectrum.

1. Introduction
Graphene is a two-dimensional hexagonal lattice of carbon atoms. Electronic properties of pristine (or free standing) graphene have been extensively studied in recent years, mainly because of its unusual properties following from specific electronic states described by the Dirac model [1–5]. It has been shown that the electronic properties can be strongly modified when graphene is decorated (or functionalized) with various adatoms or molecules attached to its surface or to edges in the case of graphene stripes and nanoribbons [6–11].

Other possibilities of a significant modification of graphene electronic and magnetic properties appear in hybrid systems based on graphene deposited on various substrates (e.g. on transition metal dichalcogenides or ferromagnetic thin films) [12–20]. Such systems are currently of great interest both experimental and theoretical, mainly because of magnetic and spin–orbit proximity effects responsible for magnetic moment and enhanced spin–orbit interaction in the graphene layer. This, in turn, opens possibilities of spin–orbit driven phenomena in graphene-based hybrid structures at room temperatures [7, 12, 14, 19, 21]. The high-temperature experimental realizations of anomalous and spin Hall effects as well as current-induced spin polarization (or Edelstein effect) make the graphene-based structures active elements of future spintronics and spin-orbitronics devices – together with other 2D crystals, semiconductor heterostructures, and junctions of oxide perovskites [22].

Hexagonal two-dimensional crystals with their prominent examples such as graphene and transition metal dichalcogenides with broken inversion symmetry are currently studied very intensively, especially in the context of so-called valleytronics and also valley-based optoelectronics [23–33]. An important property of such systems is the presence of two inequivalent ($K$ and $K'$) valleys in the corresponding electronic spectrum. Interestingly, it turned out that the valley degree of freedom can be controlled not only by circularly polarized light, but also with external magnetic and electric fields. Moreover, very promising for applications seems to be the coupling of valley and spin degrees of freedom due to spin–orbit interaction [34, 35]. Owing to this one may expect, among others, a certain enhancement of the spin and valley polarization lifetimes and also manipulation of the spin degree of freedom by valley properties. This, in turn, allows to conceive a new generation of spintronic devices which are based on chargeless and nondissipative currents.

An important issue is the pure electrical generation and detection of valley and spin currents. This can be
A Dyrdał and J Barnaś realized via the valley and spin Hall effects as well as their inverse counterparts. In systems with a net magnetization one can also observe the anomalous Hall effect. In high quality samples (free of impurities and other structural defects), these effects are determined by Berry curvature of the electronic bands and reflect topological properties of the systems [36–38]. Thus, detailed analysis of all the Hall effects in graphene-based hybrid structures is crucial for their proper understanding.

In this paper we consider two kinds of hybrid structures: (i) graphene on a few atomic monolayers of boron nitride (BN) deposited on a ferromagnetic metal like Co or Ni, and (ii) graphene deposited directly on a ferromagnetic insulating substrate (YIG). In the former case the proximity-induced exchange interaction strongly depends on the number \( n \) of atomic planes of BN, and disappears already for \( n = 4 \) such atomic planes. In the latter case, in turn, the graphene layer is deposited directly on the ferromagnetic substrate, so the exchange interaction is rather direct. Importantly, BN is a wide-gap semiconductor and therefore plays a role of energy barrier for the low-energy electronic states in graphene.

The spin–orbit and exchange-interaction driven phenomena in graphene-based hybrid structures are studied within the linear response theory and Green function formalism. To describe these phenomena theoretically we make use of the low-energy effective Hamiltonians which have been obtained recently from results of \textit{ab initio} calculations [13, 14, 18]. Because transport properties of graphene close to the charge neutrality point are determined mainly by electrons in the vicinity of Dirac points, we assume a minimal \( p_z \) model that describes electronic and spin transport properties related to the low-energy electronic states of graphene and also takes into account the proximity-induced effects.

A general low-energy Hamiltonian describing electronic states in both (\( K \) and \( K' \)) valleys in the systems under consideration includes four terms [18],

\[ H = \sum_{\alpha} \left( \begin{array}{cc} 0 & \chi_{\alpha} \rho \sigma \frac{1}{2} \left( \gamma_5 P_z \sigma \right) \div \gamma_5 P_z \sigma \frac{1}{2} \left( \gamma_5 P_z \sigma \right) \right) \begin{pmatrix} \psi_\alpha \rangle \langle \psi_\alpha \rangle \end{pmatrix} + \text{terms related to exchange interaction} \]

Figure 1. Schematic of the system under consideration. Graphene is deposited either directly on a magnetic substrate (YIG) or is separated from the magnetic substrate (Co, Ni) by a few atomic planes of another hexagonal crystal (BN). The underlayer assures the exchange field and staggered potential acting on the graphene and also gives rise to the spin–orbit interaction of Rashba type. Owing to this, one may observe the Hall effects listed at the bottom of the figure.

2. Theoretical background

2.1. Model

We consider graphene either deposited directly on a magnetic substrate, or separated from the magnetic substrate by a few atomic layers of another two-dimensional crystal (e.g. BN), as shown schematically in figure 1. The influence of the substrate on magnetic and electronic properties of graphene will be taken into account in terms of certain effective Hamiltonians which have been obtained recently from results of \textit{ab initio} calculations [13, 14, 18]. Because transport properties of graphene close to the charge neutrality point are determined mainly by electrons in the vicinity of Dirac points, we assume a minimal \( p_z \) model that describes electronic and spin transport properties related to the low-energy electronic states of graphene and also takes into account the proximity-induced effects.

A general low-energy Hamiltonian describing electronic states in both (\( K \) and \( K' \)) valleys in the systems under consideration includes four terms [18],
\[ H^{K(K')} = H_0^{K(K')} + H_{\Delta}^{K(K')} + H_{\mathrm{EX}}^{K(K')} + H_{R}^{K(K')} \]  
(1)

The first term of the above Hamiltonian describes kinetic energy near the \( K \) and \( K' \) points [47],

\[ H_0^{K(K')} = \nu(\pm k_x \sigma_x + k_y \sigma_y) s_0, \]  
(2)

where \( k_x \) and \( k_y \) are the in-plane wavevector components, \( \nu = \hbar v_F \) with \( v_F \) denoting the Fermi velocity, while the upper and lower signs correspond to the \( K \) and \( K' \) valleys, respectively. Apart from this, we use the notation according to which \( s_0 \) and \( \sigma \) are the unit matrix and the vector of Pauli matrices, \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \), acting in the pseudospin (sublattice) space, while \( s_0 \) and \( s \) denote the unit matrix and vector of Pauli matrices, \( s = (s_x, s_y, s_z) \), acting in the spin space. Although the Fermi velocity slightly depends on the substrate, we neglect this weak dependence and assume \( v_F \) constant, \( v_F = 0.812 \cdot 10^6 \text{ m s}^{-1} \) (see [18]).

The second term in equation (1) takes into account the fact that carbon atoms from different sublattices (A and B) can feel generally different local potentials [18, 39]. Such a staggered potential appears for instance when graphene is deposited on a 2D material substrates. Without loss of generality, we assume \( v_\nu \) electric field along the axis \( \nu \) is the Rashba parameter, and the upper/lower signs refer to the \( A \) and \( B \) sublattices, respectively.

\[ H_{\Delta}^{K(K')} = \Delta \sigma_\nu s_\nu. \]  
(3)

The third term in Hamiltonian (1) represents the proximity-induced exchange interaction between the graphene and magnetic substrate, given explicitly by the formula [18]

\[ H_{\mathrm{EX}}^{K(K')} = \frac{\lambda^A_{\mathrm{EX}}}{2}(\sigma_x - \sigma_0) s_z + \frac{\lambda^B_{\mathrm{EX}}}{2}(\sigma_y + \sigma_0) s_y, \]  
(4)

where \( \lambda^A_{\mathrm{EX}} \) and \( \lambda^B_{\mathrm{EX}} \) are the exchange parameters corresponding to the sublattices A and B, respectively. Note that in the special case of \( \lambda^A_{\mathrm{EX}} = -\lambda^B_{\mathrm{EX}} = \lambda_{\mathrm{EX}} \) one obtains the exchange Hamiltonian in the form:

\[ H_{\mathrm{EX}}^{K(K')} = \lambda_{\mathrm{EX}} \sigma_\nu s_\nu. \]

Finally, the last term in Hamiltonian (1) describes the spin–orbit interaction of Rashba type. This interaction takes the following general form [47]:

\[ H_{R}^{K(K')} = \lambda_R (\pm \sigma_x s_y - \sigma_y s_x), \]  
(5)

where \( \lambda_R \) is the Rashba parameter, and the upper/lower signs refer to the \( K \) and \( K' \) valleys. Note that the intrinsic spin–orbit interaction in graphene is very small and therefore it is neglected in our consideration.

\[ \sigma_{\nu \nu}^{\mathrm{AHE}} = \sigma_{\nu \nu}^K + \sigma_{\nu \nu}^{K'}, \]  
(6)

for the anomalous Hall effect (AHE),

\[ \sigma_{\nu \nu}^{\mathrm{VHE}} = \sigma_{\nu \nu}^K - \sigma_{\nu \nu}^{K'}, \]  
(7)

for the valley Hall effect (VHE),

\[ \sigma_{\nu \nu}^{\mathrm{SHE}} = \sigma_{\nu \nu}^K + \sigma_{\nu \nu}^{K'}, \]  
(8)

for the spin Hall effect (SHE), and

\[ \sigma_{\nu \nu}^{\mathrm{SVHE}} = \sigma_{\nu \nu}^K - \sigma_{\nu \nu}^{K'}, \]  
(9)

for the spin valley Hall effect (SVHE). Here, \( \sigma_{\nu \nu}^{K(K')} \) are contributions from the valley \( \nu (\nu = K, K') \) to the charge and spin conductivities, respectively.

Within the zero-temperature Green functions formalism and in the linear response with respect to a dynamical electric field of frequency \( \omega \) (measured in energy units), one can write the dynamical charge and spin conductivities in the form,

\[ \sigma_{\nu \nu}^{\nu} (\omega) = \frac{e^2 \hbar}{\omega} \int_0^\infty \int d\pi \int \frac{d^2 k}{(2\pi)^2} \times \text{Tr} \left\{ \tilde{\nu}_x \tilde{G}_x^\nu (\omega) \tilde{\nu}_x \tilde{G}_x^\nu (\omega + \epsilon) \right\}, \]  
(10)

\[ \sigma_{\nu \nu}^{\nu \nu} (\omega) = \frac{e \hbar}{\omega} \int_0^\infty \int d\pi \int \frac{d^2 k}{(2\pi)^2} \times \text{Tr} \left\{ \tilde{\nu}_x \tilde{\nu}_x \tilde{G}_x^\nu (\epsilon) \tilde{\nu}_x \tilde{G}_x^\nu (\epsilon + \omega) \right\}, \]  
(11)

for \( \nu = K, K' \). In the above equations \( \tilde{\nu}_x \) denote components of the velocity operator for the valley \( \nu \), and \( \tilde{\nu}_x^\nu = \frac{1}{\hbar} \frac{\partial \tilde{\nu}_x^\nu}{\partial \epsilon} \) is the relevant component of the spin current operator with \( \tilde{\nu}_x^\nu = \frac{1}{\hbar} \frac{\partial \tilde{\nu}_x^\nu}{\partial \epsilon} \) denoting the \( z \)-component of the spin operator. Furthermore, \( \tilde{G}_x^\nu (\epsilon) \) stands for the causal Green function corresponding to the appropriate Hamiltonian \( \tilde{H}^\nu \), \( \tilde{G}_x^\nu (\epsilon) = [\tilde{E} + \mu + i\hbar \tilde{\nu}_x^\nu (\epsilon)]^{-1} \), where \( \mu \) is the chemical potential and \( \delta \rightarrow 0^+ \) in the clean limit. We note that our considerations are limited to a defect-free system. However, one should bear in mind that disorder can lead to some modification of the Hall conductivities under consideration. This problem, however, is not considered here.

In the following we are interested in the dc-conductivities, so we take the limit \( \omega \rightarrow 0 \) in the above expressions. To do this we write

\[ \text{Tr} \left\{ \tilde{\nu}_x \tilde{G}_x^\nu (\epsilon + \omega) \tilde{\nu}_x \tilde{G}_x^\nu (\epsilon) \right\} = \mathcal{D}_0^\nu (\epsilon, k, \phi) + \omega \mathcal{D}_1^\nu (\epsilon, k, \phi) + \ldots, \]  
(12)

\[ \text{Tr} \left\{ \tilde{\nu}_x \tilde{\nu}_x \tilde{G}_x^\nu (\epsilon + \omega) \tilde{\nu}_x \tilde{G}_x^\nu (\epsilon) \right\} = \mathcal{D}_0^{\nu \nu} (\epsilon, k, \phi) + \omega \mathcal{D}_1^{\nu \nu} (\epsilon, k, \phi) + \ldots, \]  
(13)

where \( \mathcal{G}_x^\nu \) stands for a nominator of the Green function, \( \phi \) is the angle between the wavevector \( k \) and the axis \( x \), and the terms of higher order in \( \omega \) have been omitted as their contribution vanishes in the limit of \( \omega \rightarrow 0 \).
Upon calculating the trace one finds \( D_{\omega}^\nu(\epsilon, k, \phi) = 0 \) and \( D_{\omega}^{\nu\nu}(\epsilon, k, \phi) = 0 \). Thus, in the limit of \( \omega \to 0 \) the expressions (10) and (11) take the form

\[
\sigma^\nu_{xy} = \frac{e^2}{h} \int d\epsilon \int dk \mathcal{F}^\nu(\epsilon, k), \quad (14)
\]

\[
\sigma^{\nu\nu}_{xy} = \frac{e^2}{h} \int d\epsilon \int dk \mathcal{F}^{\nu\nu}(\epsilon, k), \quad (15)
\]

where the functions \( \mathcal{F}^\nu(\epsilon, k) \) and \( \mathcal{F}^{\nu\nu}(\epsilon, k) \) are defined as

\[
\mathcal{F}^\nu(\epsilon, k) = \frac{\mathcal{I}^\nu(\epsilon, k)}{\prod_{l=1}^{4}[\epsilon + \mu - E_l + i\delta \text{sgn}(\epsilon)]^2}, \quad (16)
\]

\[
\mathcal{F}^{\nu\nu}(\epsilon, k) = \frac{\mathcal{I}^{\nu\nu}(\epsilon, k)}{\prod_{l=1}^{4}[\epsilon + \mu - E_l + i\delta \text{sgn}(\epsilon)]^2}. \quad (17)
\]

Here, \( E_l \) (\( l = 1 - 4 \)) denote the four eigenmodes (subbands) of the relevant Hamiltonian, and we introduced the following notation:

\[
\mathcal{I}^\nu(\epsilon, k) = \int d\phi \mathcal{D}^\nu(\epsilon, k, \phi), \quad (18)
\]

\[
\mathcal{I}^{\nu\nu}(\epsilon, k) = \int d\phi \mathcal{D}^{\nu\nu}(\epsilon, k, \phi). \quad (19)
\]

The integration over \( \epsilon \) in equations (14) and (15) can be performed in terms of the theorem of residues. As a result one finds

\[
\sigma^\nu_{xy} = \frac{e^2}{h} \frac{1}{(2\pi)^2} \sum_{\nu=1}^{4} \int dk k R^\nu_k f(E_k), \quad (20)
\]

\[
\sigma^{\nu\nu}_{xy} = \frac{e^2}{h} \frac{1}{(2\pi)^2} \sum_{\nu=1}^{4} \int dk k R^{\nu\nu}_k f(E_k), \quad (21)
\]

for \( \nu = K, K' \). Here, \( f(E) \) is the Fermi distribution function, while \( R^\nu_k \) and \( R^{\nu\nu}_k \) denote the residua (multiplied by the factor \( 2\pi i \)) of the functions \( \mathcal{F}^\nu(\epsilon, k) \) and \( \mathcal{F}^{\nu\nu}(\epsilon, k) \), respectively, taken at \( \epsilon = E_l - \mu \).

Since we consider here only intrinsic (topological) contributions to the anomalous and valley Hall effects, one can express equation (20) alternatively in terms of the Berry curvature of the electronic bands corresponding to the valley \( \nu \),

\[
\sigma^\nu_{xy} = \frac{e^2}{h} \sum_{l=1}^{4} \int \frac{dk k}{(2\pi)^2} \Omega^\nu_l f(E_l),
\]

where \( \Omega^\nu_l \) is the \( z \) component of the Berry curvature for the \( l \)th subband, calculated in the vicinity of the point \( \nu \), while \( \tilde{\Omega}^\nu_l \) is the Berry curvature integrated over the angle \( \phi, \tilde{\Omega}^\nu_l = \int d\phi \Omega^\nu_l \). Thus, the Berry curvature can be related to the residua \( R^\nu_k \) as \( \tilde{\Omega}^\nu_l = 2\pi i R^\nu_k \). The correspondence between Kubo formulation and the approach based on topological invariants has been shown by Thouless et al. [48, 49] and then it was widely discussed in the literature (see review papers [37, 50]). Therefore, we only comment here that in the case of

\[
\Delta_{\nu}(\epsilon) = \frac{i}{2} \sum_{l=1}^{4}[\epsilon + \mu - E_l + i\delta \text{sgn}(\epsilon)]^2.
\]

Here, \( \Delta_{\nu}(\epsilon) \) and \( \lambda_{\nu\nu}(\epsilon) \) denote the residua of the functions \( \mathcal{F}^\nu(\epsilon, k) \) and \( \mathcal{F}^{\nu\nu}(\epsilon, k) \), respectively, taken at \( \epsilon = \tilde{\epsilon} \) and \( \epsilon = \tilde{\epsilon} + \Delta_{\nu}(\epsilon) \).

Therefore, we only comment here that in the case of

\[
\text{Table 1. Parameters describing graphene(Gr)-based hybrid systems under considerations, taken from [18].}
\]

| \( n \) | \( \Delta \) (meV) | \( \lambda_{12} \) (meV) | \( \lambda_{13} \) (meV) |
|---|---|---|---|
| Gr/BN/Co | 1 | 19.25 | -3.14 | 8.59 |
| 2 | 36.44 | 0.097 | -9.81 |
| 3 | 38.96 | -0.005 | 0.018 |
| Gr/BN/Ni | 1 | 22.86 | -1.40 | 7.78 |
| 2 | 42.04 | 0.068 | -3.38 |
| 3 | 40.57 | -0.003 | 0.017 |

AHE and VHE, the conductivity may be nonzero even if the energy bands are described by the zero Chern number (Berry phase). This is because the local Berry curvature may be nonzero and can give rise to the anomalous or valley Hall conductivity.

Equations (20)–(22) are our general formulas which can be used to determine all the four Hall conductivities. These formulas will be applied in the following to specific hybrid systems under consideration.

3. Graphene/BN(n)/Co(Ni)

Consider first graphene on a few (\( n \)) atomic planes of hexagonal BN which is deposited on ferromagnetic Co or Ni. Since BN has a wide energy gap, it can be considered as an insulating barrier. Thus, the influence of Co (or Ni) on transport properties of graphene in the low-energy region is determined mainly by exchange interaction between graphene end Co (Ni) through the BN layer. It has been concluded from \textit{ab initio} calculations that the Rashba interaction in graphene/BN/Co(Ni) hybrid system is much smaller than the exchange term and can be ruled out [18]. Therefore, we consider the limit of vanishing Rashba interaction. The relevant parameters extracted from \textit{ab initio} calculations for the graphene/BN/Co(Ni) systems by Zollner \textit{et al.} [18] are given in table 1. These parameters will be used below in our model calculations.

When the Rashba coupling disappears, Hamiltonian for the graphene/BN/Co(Ni) hybrid system can be reduced to the form

\[
H^{K(K')} = H_0^{K(K')} + H_\Delta^{K(K')} + H^{EX}_{K(K')}. \quad (23)
\]

The corresponding dispersion relations for the K valley in case of graphene/BN/Co are shown in figure 2 (top panel) for \( n = 1, n = 2 \) and \( n = 3 \) monolayers of BN. Splitting of the conduction and valence bands due to exchange interaction, clearly seen for \( n = 1 \) (figure 2(a)), becomes reduced for \( n = 2 \) (figure 2(b)) and is negligible for \( n = 3 \) (figure 2(c)). This is a consequence of reduced exchange interaction when the number of atomic planes of BN increases. Note, splitting of the valence band is remarkably larger than that of the conduction band. Another interesting property of the spectrum is a relatively wide energy gap (40–60 meV) due to the sublattice symmetry breaking, and width of this gap depends on the number \( n \) of BN atomic monolayers. This orbital
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Gap is a consequence of the presence of BN, and its width increases with increasing number \( n \) of BN monolayers. Interestingly, the gap is much wider than the spin–orbit gap in freestanding graphene, where it is negligible due to a very small intrinsic spin–orbit interaction.

Berry curvature integrated over the angle \( \phi \) is shown in figure 2 (bottom panel) for \( n = 1 \), \( n = 3 \), and for both \( K \) and \( \bar{K} \) valleys. This figure clearly shows that the curvature of electronic bands in the \( K \) valley is opposite to the corresponding curvature in the \( \bar{K} \) valley. As a result one finds \( \sigma_{xy}^{\text{VHE}} = -e \lambda_{\text{EX}} \hbar \), and from similar reasons also the SVHE is nonzero.

3.1. Valley Hall effect

Due to the opposite Berry curvature of the electronic bands in the \( K \) and \( \bar{K} \) valleys, electrons from both valleys are deflected to opposite edges, giving rise to a nonzero valley Hall conductivity, see equation (7).

Simple analytical results can be derived in a specific case of \( \lambda_{\text{EX}}^A = 0 \). The corresponding dispersion curves around the \( K \) point are shown in figure 2(d). Note, the conduction band is then degenerate at \( k = 0 \). When \( \lambda_{\text{EX}}^A = 0 \), analytical calculations show that the valley Hall conductivity depends on the Fermi level \( \mu \), and bearing in mind that \( \Delta > |\lambda_{\text{EX}}^B| \), this dependence can be written as follows:

(i) \( -\Delta + |\lambda_{\text{EX}}^B| < \mu < \Delta \) (Fermi level inside the gap):

\[
\sigma_{xy}^{\text{VHE}} = -\frac{2e^2}{h},
\]

i.e. the valley Hall conductivity is quantized.

(ii) \( \mu > \Delta \) (Fermi level inside the conduction bands), or \( \mu < -(\Delta + |\lambda_{\text{EX}}^B|) \) (Fermi level inside the valence bands):

\[
\sigma_{xy}^{\text{VHE}} = -\frac{2\Delta + \lambda_{\text{EX}}^B}{2\mu + \lambda_{\text{EX}}^B} \left| \frac{\Delta - \lambda_{\text{EX}}^B}{2\mu - \lambda_{\text{EX}}^B} \right| \frac{e^2}{h}.
\]

(iii) \( -(\Delta + |\lambda_{\text{EX}}^B|) < \mu < -\Delta + |\lambda_{\text{EX}}^B| \):

\[
\sigma_{xy}^{\text{VHE}} = -\left( 1 + \frac{2\Delta - |\lambda_{\text{EX}}^B|}{2\mu - |\lambda_{\text{EX}}^B|} \right) \frac{e^2}{h}.
\]

In a general situation, \( \lambda_{\text{EX}}^A = 0 \), the integrals over wavevector \( k \) were calculated numerically and the valley Hall conductivity is shown in figure 3 as a function of the chemical potential \( \mu \). As follows from table 1, the parameter \( \lambda_{\text{EX}}^A \) is remarkably smaller than \( \lambda_{\text{EX}}^B \), especially for \( n = 2 \) BN planes. Thus, the analytical results for VHE, obtained with \( \lambda_{\text{EX}}^A = 0 \), fit well to the corresponding numerical results obtained for the realistic

Figure 2. Energy dispersion curves around the \( K \) point for \( n = 1 \) (a), \( n = 2 \) (b), and \( n = 3 \) (c) atomic planes of BN and other parameters parameters as presented in the text and in the table 1. Dispersion curves in the special case of \( \lambda_{\text{EX}}^A = 0 \) are shown in (d).
values of $\lambda_{\text{EX}}^A$ taken from table 1. Therefore, we do not show the results for $\lambda_{\text{EX}}^A = 0$ in figure 3.

The valley Hall conductivity is quantized and universal when the Fermi level is in the gap, where $\sigma_{xy}^{\text{HVF}} = -\frac{e^2}{h}$. The absolute value of the conductivity for $\mu$ outside the gap is reduced with increasing $|\mu|$. The kinks appear at the points where the Fermi level crosses the edges of the conduction or valence bands, and appear in the presence of exchange splitting of the bands. Note, such a splitting disappears for $n = 3$ monolayers of BN, where the exchange interaction is vanishingly small. The kinks for positive $\mu$ are less pronounced as the exchange-induced splitting of the conduction band is remarkably smaller.

### 3.2. Spin valley Hall effect

As already mentioned above, the spin Hall effect vanishes in graphene/BN/Co (Ni) systems due to vanishingly small Rashba interaction. Strictly speaking, contributions to the spin Hall conductivity from individual valleys are nonzero, however they cancel each other as the spin currents associated with the $K$ and $K'$ valleys are opposite. Thus, similarly to the valley Hall effect, one can define the spin valley Hall effect as the difference of spin currents from the $K$ and $K'$ valleys, see equation (9) and also [51]. This quantity is generally nonzero, and indicates that the net spins from the $K$ and $K'$ valleys are deflected to the opposite edges.

Similarly as in the previous section we analyse the full model with the realistic parameters $\lambda_{\text{EX}}^A$ (see table 1), as well as the limit $\lambda_{\text{EX}}^A = 0$. For vanishing $\lambda_{\text{EX}}^A$ it is possible to find analytical solutions for the spin valley Hall conductivity:

(i) $\mu > \Delta:

$$\sigma_{xy}^{\text{SVHE}} = \frac{e}{2\pi} \left( \frac{2\Delta - \lambda_{\text{EX}}^B}{|2\mu - \lambda_{\text{EX}}^B|} - \frac{2\Delta + \lambda_{\text{EX}}^B}{|2\mu + \lambda_{\text{EX}}^B|} \right).$$ \tag{27}

(ii) $-\Delta + |\lambda_{\text{EX}}^B| < \mu < \Delta$ (Fermi level is in the gap):

$$\sigma_{xy}^{\text{SVHE}} = \frac{e}{2\pi} \left( \frac{2\Delta - \lambda_{\text{EX}}^B}{|2\mu - \lambda_{\text{EX}}^B|} - \frac{2\Delta + \lambda_{\text{EX}}^B}{|2\mu + \lambda_{\text{EX}}^B|} \right).$$

Numerical results on the spin valley Hall conductivity are presented in figure 4 for $n = 1$, $n = 2$ and $n = 3$, and for both the realistic values of $\lambda_{\text{EX}}^A$ and for $\lambda_{\text{EX}}^A = 0$. The spin valley Hall conductivity vanishes for the Fermi level in the gap. To understand this we note first that the exchange-splitting of conduction (and also valence) bands is the same in the $K$ and $K'$ valleys. Since the two valence subbands in an individual valley correspond to opposite spin orientations, their contributions to the spin current exactly cancel each other when the Fermi level is in the energy gap. A nonzero spin current appears then when the Fermi level crosses the bottom edge of the lower conduction subband or top edge of the higher valence subband. When $|\mu|$ grows further, the magnitude of spin valley Hall conductivity decreases due to compensating contribution from the second conduction (valence) subband.

Note, the spin valley Hall conductivity for $n = 2$ atomic planes of BN has reversed sign in major part of $\mu$ due to reversed sign of the exchange parameter in comparison to that for $n = 1$ (see table 1). Apart from this, the magnitude of spin valley Hall conductivity for $n = 3$ is roughly three orders of magnitude smaller than for $n = 1$. This is due to a very small exchange coupling parameter for $n = 3$. Interestingly, the difference between the analytical results for $\lambda_{\text{EX}}^A = 0$ and the
results for realistic $\lambda_{\text{EX}}$ is now more remarkable, as follows from figure 4. This difference appears mainly for $n = 1$ and $n = 3$, while it is negligible for $n = 2$ since $\lambda_{\text{EX}}^A / \lambda_{\text{EX}}^B \ll 1$.

4. Graphene on a magnetic insulating substrate

Now we consider graphene deposited directly on a magnetic insulating substrate. An important example of such a hybrid system is graphene deposited on YIG, where large anomalous Hall effect at room temperature has been measured recently [14, 19]. In this particular case the second term of Hamiltonian (1), corresponding to the orbital gap, is absent. However, the coexistence of proximity-induced exchange field and Rashba spin–orbit coupling is essential. Therefore, Hamiltonian (1) for the graphene/YIG system can be reduced to the following one [13, 14]:

$$H^{K(\text{K})} = H_0^{K(\text{K})} + H_{\text{EX}}^{K(\text{K})} + H_R^{K(\text{K})}. \quad (31)$$

Moreover, one may assume $\lambda_{\text{EX}}^A = -\lambda_{\text{EX}}^B = \lambda_{\text{EX}}$ in this particular case, so the relevant exchange Hamiltonian takes the simple form

$$H_{\text{EX}}^{K(\text{K})} = \lambda_{\text{EX}} \sigma_\phi z. \quad (32)$$

Figure 5 presents the dispersion curves for the graphene/YIG structure (top panel). The Rashba coupling was assumed there constant while the exchange parameter was changed (as indicated) from weak to strong coupling limit. Interestingly, when the exchange coupling is small, there is no energy gap in the spectrum, and the gap is created when the exchange interaction is sufficiently strong. Apart from this, minima (maxima) of the conduction (valence) bands are shifted away from the Dirac points. The bottom panel in figure 5 shows the Berry curvature corresponding to the bands displayed in the top panel. The Berry curvature for the $K$ point (not shown) is the same as that for the $K'$ point. Due to this, both VHE and SVHE are absent. However, AHE and SHE conductivities do not vanish due to Rashba spin–orbit coupling, and both can be found following the approach described in section 2.
4.1. Spin Hall effect

To find the spin Hall conductivity we make use of equation (21). The corresponding residua can be easily evaluated and are given by the expressions

\[ R^{\text{K-i}}_{\mu\lambda\lambda} = \pi \lambda_{\mu\lambda\lambda} \left( \frac{\lambda_{\mu} + \lambda_{\lambda} \lambda_{\lambda} + \sqrt{\lambda_{\mu}^2 + \lambda_{\lambda}^2 \lambda_{\lambda}^2}}{\lambda_{\mu} + \lambda_{\lambda} \lambda_{\lambda} + \sqrt{\lambda_{\mu}^2 + \lambda_{\lambda}^2 \lambda_{\lambda}^2}} \right)^{3/2}, \tag{33} \]

\[ R^{\text{K-i}}_{\lambda\lambda\lambda} = -\pi \lambda_{\lambda\lambda\lambda} \left( \frac{\lambda_{\lambda} + \lambda_{\lambda} \lambda_{\lambda} + \sqrt{\lambda_{\lambda}^2 + \lambda_{\lambda}^2 \lambda_{\lambda}^2}}{\lambda_{\lambda} + \lambda_{\lambda} \lambda_{\lambda} + \sqrt{\lambda_{\lambda}^2 + \lambda_{\lambda}^2 \lambda_{\lambda}^2}} \right)^{3/2}, \tag{34} \]

Taking the above formulas into account, one can find explicit expressions for the spin Hall conductivity, which are valid in the corresponding regions of the chemical potential, as described below. These regions can be easily identified when looking at the dispersion curves in figure 5.

(i) \( |\mu| > 4 \lambda_{\mu}^2 + \lambda_{\lambda}^2 \lambda_{\lambda}^2 \):

\[ \sigma_{\alpha\beta}^{\text{SHE}} = \pi \lambda_{\mu\lambda\lambda} \left( \frac{k_{3+}^2}{\xi_{3+}^2} - \frac{k_{3-}^2}{\xi_{3-}^2} \right), \]

\[ \pm \frac{e}{4\pi} \lambda_{\mu\lambda\lambda} \left( \lambda_{\mu}^2 + \lambda_{\lambda}^2 \lambda_{\lambda}^2 \right)^{3/2} \left( \frac{1}{\xi_{3+}} - \frac{1}{\xi_{3-}} \right), \tag{35} \]

with the upper sign for \( \mu < 0 \) and lower for \( \mu > 0 \).

(ii) \( 4 \lambda_{\mu}^2 + \lambda_{\lambda}^2 > |\mu| > \lambda_{\lambda}^2 \lambda_{\lambda}^2 \):

\[ \sigma_{\alpha\beta}^{\text{SHE}} = \pm \frac{e}{8\pi} \lambda_{\mu\lambda\lambda} \left( \frac{k_{3+}^2}{\xi_{3+}^2} - \frac{k_{3-}^2}{\xi_{3-}^2} \right) \]

\[ \pm \frac{e}{4\pi} \lambda_{\mu\lambda\lambda} \left( \lambda_{\mu}^2 + \lambda_{\lambda}^2 \lambda_{\lambda}^2 \right)^{3/2} \left( \frac{1}{\xi_{3+}} - \frac{1}{\xi_{3-}} \right), \tag{36} \]

with the upper sign for \( \mu < 0 \) and lower for \( \mu > 0 \).

(iii) \( \lambda_{\lambda}^2 \lambda_{\lambda}^2 > |\mu| > \lambda_{\mu}^2 \lambda_{\mu}^2 \):

\[ \sigma_{\alpha\beta}^{\text{SHE}} = \pm \frac{e}{8\pi} \lambda_{\mu\lambda\lambda} \left( \frac{k_{3+}^2}{\xi_{3+}^2} - \frac{k_{3-}^2}{\xi_{3-}^2} \right) \]

\[ \pm \frac{e}{4\pi} \lambda_{\mu\lambda\lambda} \left( \lambda_{\mu}^2 + \lambda_{\lambda}^2 \lambda_{\lambda}^2 \right)^{3/2} \left( \frac{1}{\xi_{3+}} - \frac{1}{\xi_{3-}} \right), \tag{37} \]

with the upper sign for \( \mu < 0 \) and lower for \( \mu > 0 \).

(iv) \( \lambda_{\mu}^2 \lambda_{\mu}^2 > |\mu| > \lambda_{\lambda}^2 \lambda_{\lambda}^2 \) (i.e. in the gap of electronic spectrum):

\[ \sigma_{\alpha\beta}^{\text{SHE}} = 0, \tag{38} \]

i.e. the spin Hall conductivity vanishes.

In the above equations we introduced the notation:

\[ k_{3\pm} = \pm \frac{1}{2} \sqrt{\lambda_{\mu}^2 + \mu^2 \pm 2 \mu \lambda_{\lambda}^2} \lambda_{\lambda}^2 \lambda_{\lambda}^2 - \lambda_{\mu}^2 \lambda_{\mu}^2 \]

and

\[ \xi_{3\pm} = \pm \sqrt{\lambda_{\mu}^2 + k_{3\pm}^2 \lambda_{\lambda}^2 \lambda_{\lambda}^2}. \]

Figure 6. Spin Hall conductivity in the graphene/YIG system as a function of chemical potential and exchange parameter for fixed Rashba parameter \( \lambda_{\mu} = 10 \text{ meV} \) (a) and as a function of chemical potential and Rashba parameter for fixed exchange parameter \( \lambda_{\lambda} = 10 \text{ meV} \) (c). (b) and (d) represent cross-sections of the density plots in (a) and (c), respectively.
Variation of the spin Hall conductivity with the chemical potential $\mu$ and Rashba and exchange parameters is shown in figure 6. For small values of the exchange parameter, the spin Hall conductivity depends on the chemical potential in a similar way as in graphene on a nonmagnetic substrate [52]. However, when the exchange coupling increases, the spin Hall conductivity vanishes in the energy gap created by the exchange interaction around $\mu = 0$, where $\sigma_{xy}^{\text{SHE}} = 0$. This is clearly seen in figures 6(b) and (c), where the platos correspond to the zero spin Hall conductivity in the gap. Vanishing of spin Hall conductivity in the gap is a consequence of the compensation of the contributions from the two occupied valence subbands which correspond to opposite spin orientations. Width of a given plato depends on the strengths of Rashba and exchange parameters. Outside the platos, the absolute value of $\sigma_{xy}^{\text{SHE}}$ grows up and upon reaching a maximum decreases with a further increase in $|\mu|$, tending to a universal value $e^2/4\pi$.

### 4.2. Anomalous Hall effect

The anomalous Hall conductivity can be calculated in a similar way as the spin Hall conductivity. The corresponding formulas for the residua, and thus also for the anomalous Hall conductivity, are rather cumbersome, so they are not presented here. Instead, we show in figure 7 only numerical results. First, one can note that the anomalous Hall conductivity disappears for vanishing Rashba coupling. It also vanishes when the exchange coupling is zero since the system is then nonmagnetic. Indeed, to have a nonzero anomalous Hall conductivity we need simultaneously a nonzero spin–orbit coupling (of Rashba form in the case under consideration) and a nonzero magnetic moment of the system, which here appears due to exchange coupling to the magnetic substrate. The most interesting feature of the AHE is the quantized and universal value of the corresponding Hall conductivity for chemical potentials in the gap formed around $\mu = 0$ due to the exchange coupling, where $\sigma_{xy}^{\text{AHE}} = -2e^2/h$. This quantized value is of intrinsic (topological) origin, and is a consequence of the fact that the Berry curvatures of the bands in the $K$ and $K'$ valleys are the same.

### 5. Summary

In this paper we analyzed graphene based hybrid systems, more specifically graphene deposited on magnetic substrates. The key objective was to study the influence of proximity effects – especially of the spin–orbit interaction of Rashba type, staggered potential, and the proximity-induced exchange interaction. Two kinds of systems were considered: (i) graphene deposited on a few atomic monolayers of boron nitride, which in turn was deposited on a magnetic substrate (Co or Ni), and (ii) graphene deposited directly on a magnetic (insulating) substrate like YIG. To describe these systems we assumed the model Hamiltonians which were proposed recently on the basis of results obtained from \textit{ab initio} calculations.
Our main interest was in the spin, anomalous and valley Hall effects. In addition, we also introduced the spin valley Hall effect. The corresponding conductivities were calculated in the linear response regime and within the Green function formalism. In the case of graphen/BN/Co(Ni) hybrid system, the strength of the corresponding conductivities were calculated in the linear response regime and also in a nonzero spin valley Hall effect. These effects are absent in the case when graphene is deposited directly on YIG. However, anomalous and spin Hall effects can be then observed, with the universal quantized value of the Fermi level in the energy gap. This universal value follows from the topological properties and nonzero Berry curvature. We also note that our considerations were limited to pristine systems, with no electron scattering. However, one should note that electron scattering, especially inter-valley scattering, plays an important role in VHE [53].

Acknowledgments

This work has been supported by the National Science Center in Poland as research project No. DEC-2013/10/M/ST3/00488 and by the Polish Ministry of Science and Higher Education (AD) through the research project ‘Juventus Plus’ in years 2015–2017 (project No. 0083/IP3/2015/73). A D also acknowledges support from the Foundation for Polish Science (FNP).

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References

[1] Geim A K and Novoselov K S 2007 Nat. Mater. 6 183
[2] Katsnelson M I 2007 Mater. Today 10 20
[3] Neto A H C, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 Rev. Mod. Phys. 81 109
[4] Abergel D S L, Apalkov V, Berahevich J, Ziegler K and Chakraborty T 2010 Adv. Phys. 59 261
[5] Credi A, Nikolic B K, Garcia J H and Roche S 2016 Rev. Nuovo Cimento 39 587
[6] Roche S et al 2015 2D Mater. 2 030202
[7] Gmitra M, Kochan D and Fabian J 2013 Phys. Rev. Lett. 110 246602
[8] Balakrishnan J, Koon G K W, Iaiswal M, Neto A H C and Ozyilmaz B 2013 Nat. Phys. 9 284
[9] Irmer S, Frank T, Putz T, Gmitra M, Kochan D and Fabian J 2015 Phys. Rev. B 91 115411
[10] Soriano D, Van Tuan D, Dubois S M M, Gmitra M, Cummings A W, Kochan D, Oertmann F, Chartier J-C, Fabian J and Roche S 2015 2D Mater. 2 022002
[11] Avsar A, Lee J H, Koon G K W and Ozyilmaz B 2015 2D Mater. 2 044009
[12] Zberezki C, Swirkowicz R, Wierzbicki M and Barnaś J 2016 Phys. Chem. Chem. Phys. 18 181246
[13] Qiao Z, Ren W, Chen H, Bellaische L, Zhang Z, MacDonald A H and Niu Q 2014 Phys. Rev. Lett. 112 116404
[14] Wang Z, Tang C, Sachs R, Barlas Y and Shi J 2015 Phys. Rev. Lett. 114 036603
[15] Gmitra M and Fabian J 2015 Phys. Rev. B 92 155403
[16] Gmitra M, Kochan D, Hogl P and Fabian J 2016 Phys. Rev. B 93 155404
[17] Yang B, Tu M-F, Kim J, Wu Y, Wang H, Alieza J, Wu R, Bockrath M and Shi J 2016 2D Mater. 3 033012
[18] Zollner K, Gmitra M, Frank T and Fabian J 2016 Phys. Rev. B 94 155441
[19] Leutnantsmeyer J C, Kaverzin A A, Wojtaszek M and van Wees B J 2017 2D Mater. 4 014001
[20] Hallal A, Fatima Ibrahim F, Yang H, Roche S and Chshiev M 2017 2D Mater. 4 025074
[21] Mendes J B S et al 2015 Phys. Rev. Lett. 115 226601
[22] Soumyanarayanan A, Reyren N, Albert Fert A and Panagopoulos C 2016 Nature 539 509
[23] Yao W, Xiao D and Niu Q 2008 Phys. Rev. B 77 235406
[24] Xiao D, Liu G-B, Feng W, Xu X and Yao W 2012 Phys. Rev. Lett. 108 196802
[25] Ezawa M 2013 Phys. Rev. B 88 161406
[26] Ezawa M 2014 Phys. Rev. B 89 195413
[27] Yamamoto M, Shimazaki Y, Borzenets I V and Tarucha S 2015 J. Phys. Soc. Japan 84 121006
[28] Ezawa M 2015 J. Phys. Soc. Japan 84 121003
[29] Song Z, Quhe R, Liu S, Li Y, Feng J, Yang Y, Lu J and Yang J 2015 Sci. Rep. 5 13906
[30] Song Z et al 2017 Nano Lett. 17 2079
[31] Aivazian G, Gong Z, Jones A M, Chu R-L, Yan J, Mandrus D G, Zhang Ch, Cobden D, Yao W and Xu X 2015 Nat. Phys. 11 148
[32] Schaibley J R, Yu H, Clark G, Rivera F, Ross J S, Seyler K L, Yao W and Xu X 2016 Nat. Rev. Mater. 1 11
[33] Zhang W, Qixing Wang Q, Chen Y, Wang Z and Wei A T S 2016 2D Mater. 3 022001
[34] Xu X, Yao W, Xiao D and Heintz T F 2014 Nat. Phys. 10 343
[35] Liu G-B, Xiao D, Yao Y, Xude X and Yao W 2015 Chem. Soc. Rev. 44 2643
[36] Zhang X-P, Huang Ch and Cazalilla M A 2017 2D Mater. 4 024007
[37] Berry M V 1984 Proc. R. Soc. Lond. A 392 45
[38] Xiao D, Chang M-C and Niu Q 2010 Rev. Mod. Phys. 82 1959
[39] Ezawa Z F 2008 Quantum Hall Effects: Field Theoretical Approach and Related Topics (Singapore: World Scientific)
[40] Kochan D, Irmer S and Fabian J 2017 Phys. Rev. B 93 164515
[41] Dyakonov M I and Perel V I 1971 Pisma Z. Eksp. Teor. Fiz. 13 657
[42] Dyakonov M I and Perel V I 1971 JETP Lett. 13 467
[43] Hirsch J E 1999 Phys. Rev. Lett. 83 1834
[44] Engel H A, Rasbha E I and Halperin B L 2007 Handbook of Magnetism and Advanced Magnetic Materials (Spintronics and Magnetoelectronics vol 5) ed H Kronmuller and S Parkin (New York: Wiley)
[45] Nagaosa N, Sinova J, Onoda S, MacDonald A H and Ong N P 2010 Rev. Mod. Phys. 82 1539
[46] Panagopoulos C 2016 Phys. Rev. Lett. 116 256601
[47] Qiao Z, Ren W, Chen H, Bellaische L, Zhang Z, MacDonald A H and Niu Q 2014 Phys. Rev. Lett. 112 116404