Spin Filtering in a Magnetized Zigzag Phosphorene Nanoribbon

M Ali M Keshtan and Mahdi Esmaeilzadeh
Department of Physics, Iran University of Science and Technology, Narmak, Tehran 16844, Iran

Abstract

Using the equilibrium Green's function method and applying the Landauer-Büttiker formula, the spin dependent electron transport properties of a zigzag phosphorene nanoribbon at zero temperature are studied. The depositing of two ferromagnetic strips on the edges of the nanoribbon induces exchange fields with parallel and anti-parallel configurations. An external perpendicular electric field is also applied to manipulate the spin dependent electron conductance properties. Due to the order of the zigzag phosphorene nanoribbons edge bands near zero Fermi energy, parallel and anti-parallel configurations result in different properties. For anti-parallel configuration, spin filtering only occurs in the presence of the perpendicular electric field, while in the parallel case spin filtering takes place both in the absence and in the presence of the electric field. Although spin filtering properties are invariant against the inversion of the direction of the electric field in a parallel configuration, this inversion changes the spin filtering type for anti-parallel configurations.

Introduction

Phosphorene, a novel 2D black phosphorus (BP) with a few layers, is an ambient stable van der Waals material consisting of puckered atomic honeycomb lattices of phosphorous which merges high carrier mobility with a conventional semiconductor range band gap.

Similarly to other 2D materials, armchair-PNRs (APNRs) and zigzag-PNRs (ZPNRs) are two typical crystal ribbon orientations (see figure 2(a)). Pristine APNRs are semiconductors with an indirect band gap, while their ZPNR counterparts are metal, regardless of the ribbon width. As proper candidates for field effect transistors (FETs), the effects of an external electric field on PB and PNRs have been investigated. Has been ignored the spin dependency in tight-binding Hamiltonian approximation, studying the spin-dependent band structure and the spin-dependent conductance of ZPNRs using the equilibrium Green's function method sounds like a good proposal in spintronics [1].

Theory and Method

The system structure and Hamiltonian

To study a nanoribbon junction, usually it is divided to three distinct parts, namely two steady state semi-infinite leads which are connected to an interacting center part [2]. For a phosphorene nanoribbon, with two ferromagnetic strips deposited on its edges as it is shown in figure 1, and a tunable perpendicular electric field, the effective interacting one particle Hamiltonian for electron dynamics can be written in TB approximation as

$$H = \sum_{i,\alpha}(\varepsilon_i + e\frac{l}{2}\mu_i E_z)\, c^{\dagger}_{i\alpha} c_{i\alpha} + \sum_{i,j,\alpha} t_{ij} c^{\dagger}_{i\alpha} c_{j\alpha} + M\sum_{i,\alpha} c^{\dagger}_{i\alpha}\sigma_z c_{i\alpha}, \quad (1)$$

where the summations run over the lattice sites and two spins, and $c^{\dagger}_{i\alpha}$ ($c_{i\alpha}$) is the creation (annihilation) operator of electrons with spin α at site i. In the first term, ε_i describes any static local potential except the particle potential energy induced by the applied perpendicular electric field (E_z), $-e$ is the electron charge, $l = 2.057\AA$ is the vertical distance between phosphorus atoms in two different sublattice planes and $\mu_i = \pm 1$ which is due to its up or down planar relation, respectively. The second term represents the interactions between neighbour atoms and t_{ij} is the transfer energy between sites i and j which based on proposed model with hopping integrals between five neighbour sites their magnitude are as follows: $t_1 = -1.220\,eV$, $t_2 = 3.665\,eV$, $t_3 = -0.205\,eV$, $t_4 = -0.105\,eV$ and $t_5 = -0.055\,eV$ (All of these are clarified in figure 2(b)). The third term is due to the exchange field induced by deposition of the ferromagnetic strips on the nanoribbon edges, $M = 0.2\,eV$ is the exchange field strength, and σ_z is the z component of the Pauli matrix [3, 4].

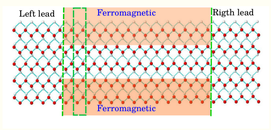


Figure 1: A $10-ZPNR$ sketch with left and right leads. Two ferromagnetic strips are deposited on the upper and lower edges of the nanoribbon. The exchange fields induced by ferromagnetic strips are normal to the phosphorene plane with parallel or anti-parallel configuration. Dashed line rectangle denotes the unit cell which is used to study band structure.

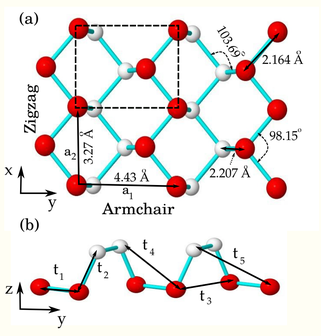


Figure 2: Crystal structure and transfer energies t_i of a single layer phosphorene for TB model. (a) Top view. (b) Side view. Red (white) balls represent phosphorous atoms in the lower (upper) layer. The dashed line rectangle denotes the primitive unit cell containing four atoms, two atoms in each layer.

The method and Formalism

To explain the band structure of the nanoribbons, the eigenvalues of the crystal Hamiltonian between Bloch sums that is $M_{\alpha,\beta}(\mathbf{k})$ must be solved [5]. In the proper orthonormal crystal basis, $M_{\alpha,\beta}(\mathbf{k})$ is given by

$$M_{\alpha,\beta}(\mathbf{k}) = \langle\phi_\alpha(\mathbf{k},\mathbf{r})|H|\phi_\beta(\mathbf{k},\mathbf{r})\rangle = -\sum_{i,j} t_{i,\alpha;j\beta}\, e^{i\mathbf{k}\cdot\mathbf{R}_{i,j}}, \quad (2)$$

where α and β stand for the intra unit cell basis sites, $\phi(\mathbf{k},\mathbf{r})$ is the Bloch wave vector, $\mathbf{k}$ is the wave vector, $\mathbf{R}_{i,j}$ indicates a Bravais lattice vector, i and j denote different unit cells and $t_{i,\alpha;j,\beta}$ are the hopping integrals between the basis site α of the unit cell i and the basis site β of the unit cell j, where they could be properly replaced by the five hopping parameters.
Using the equilibrium Green's function method and applying the Landauer-Büttiker formula [6] at zero temperature, the conductance may be written as [2]

$$G_{LR}(E_F) = \frac{e^2}{h} Tr\{\Gamma_L(E_F)\, g^r_{LR}(E_F)\, \Gamma_R(E_F)\, g^a_{RL}(E_F)\}, \quad (3)$$

where G_{LR} indicates the electron conductance from left lead to right one and E_F is the electron Fermi energy. The line width function $\Gamma_{L(R)}$ that describes the coupling between the center part of the system and the left (right) lead is given by

$$\Gamma_{L(R)}(E_F) = i\{\Sigma^r_{L(R)}(E_F) - \Sigma^a_{L(R)}(E_F)\}. \quad (4)$$

In the above equation, $\Sigma^r_{L(R)} = [\Sigma^a_{L(R)}]^{\dagger}$ is the retarded self-energy of the left (right) lead that can be calculated by an iterative method numerically [7]. In Eq. 3, the retarded Green's function of the center part could be calculated by using the following equation

$$g^r_{LR}(E_F) = (g^a_{RL})^{\dagger} = \frac{1}{(E_F + i\eta)I - H_c - \Sigma^r_L(E) - \Sigma^r_R(E)}, \quad (5)$$

where g^a_{RL} is the advanced Green's function, H_c represents the center part Hamiltonian and η is the phenomenological broadening parameter. Using Eq. 5, the density of states (DOS) is given by $DOS = -\frac{1}{\pi}\Im\{Tr[g^r_{LR}]\}$.

Results

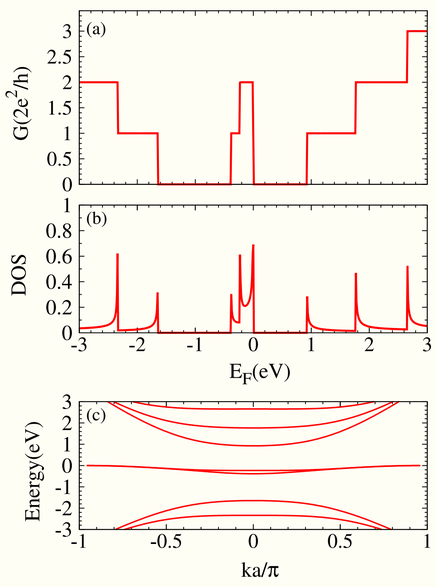


Figure 3: (a) Spin dependent conductance for both spin up and spin down; (b) density of state as a function of the Fermi energy E_F and its band structure (c) in the absence of both exchange field M and external perpendicular electric field E_z. Because of spin degeneracy, all graphs for spin up and spin down are totally coincident.

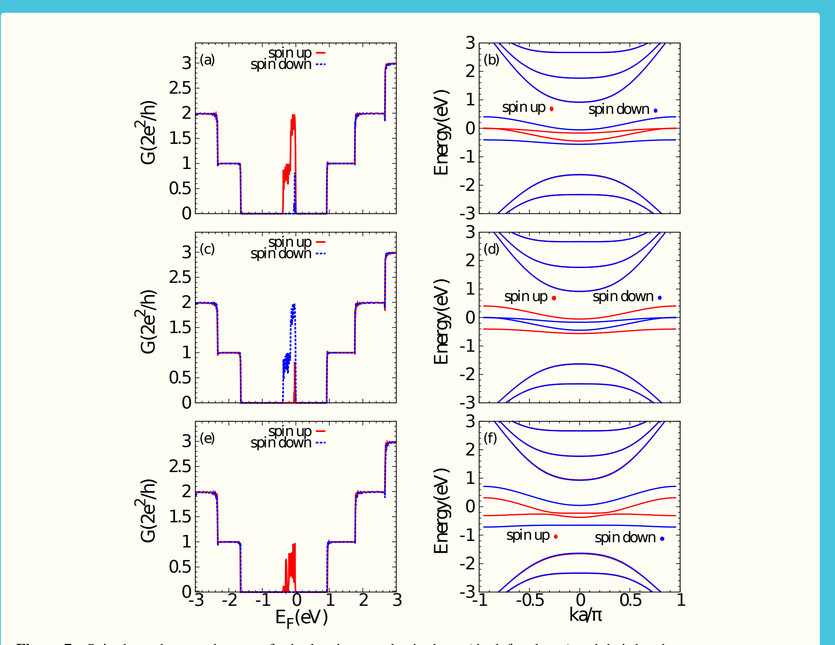


Figure 7: Spin dependent conductance for both spin up and spin down (the left column) and their band structure counterparts (the right column) in the presence of anti-parallel edges exchange fields and different external perpendicular electric fields (E_z). In the first two rows (a)-(d), the electric field strengths are the same but their directions are opposite [i.e., $eE_z = 0.2\,eV/\AA$ in (a) and (b) and $eE_z = -0.2\,eV/\AA$ in (c) and (d)]. In (e) and (f) the electric field magnitude is $eE_z = 0.5\,eV/\AA$. In all cases, except in the vicinity of zero energy, graphs for spin up and spin down are totally coincident.

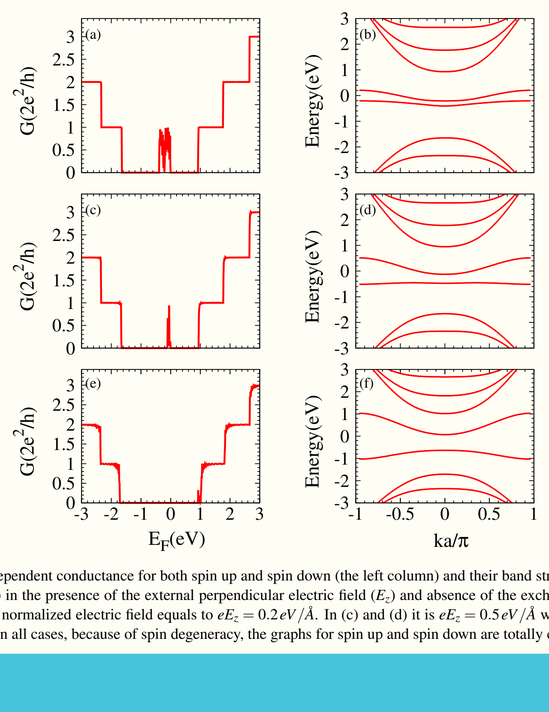


Figure 4: Spin dependent conductance for both spin up and spin down (the left column) and their band structure counterparts (the right column) in the presence of the external perpendicular electric field (E_z) and absence of the exchange field ($M = 0$). In (a) and (b), the normalized electric field equals to $eE_z = 0.2\,eV/\AA$. In (c) and (d) it is $eE_z = 0.5\,eV/\AA$ when in (e) and (f) it is $eE_z = 1\,eV/\AA$. In all cases, because of spin degeneracy, the graphs for spin up and spin down are totally coincident.

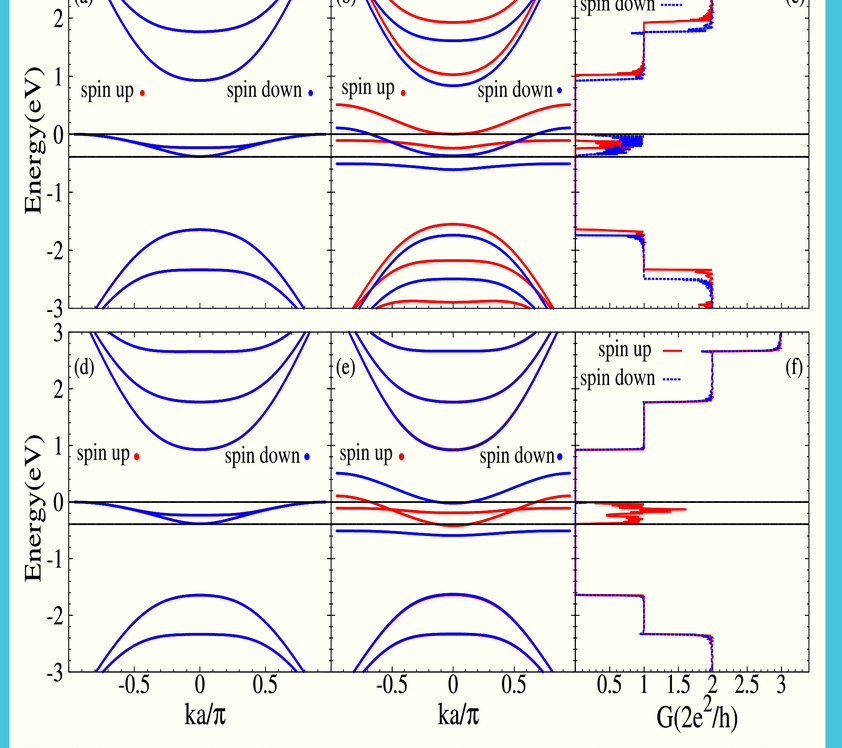


Figure 8: Correspondence of the lead band structure [(a) and (d)] with the center part band structure [(b) and (e)] to illustrate the conductance window in the vicinity of the zero Fermi energy ($-0.38\,eV < E_F < 0$). The conductance of the system (center part plus leads) is shown in (e) and (f). Here, both exchange field and external perpendicular electric field ($eE_z = 0.3\,eV/\AA$) are present. In the first row (a)-(c), the edge magnetisations are parallel while in the second row (d)-(f), they are anti-parallel. Black lines specify the boundaries of the conductance window.

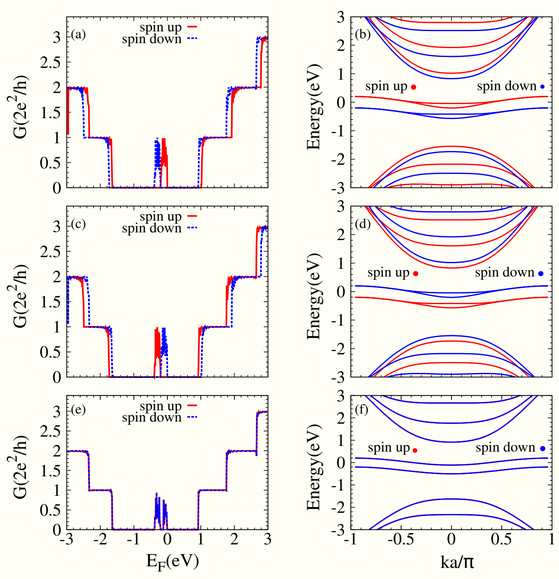


Figure 5: Spin dependent conductance for both spin up and spin down (the left column) and their band structure counterparts (the right column) in the absence of electric field ($E_z = 0$). (a) and (b) stand for parallel exchange fields exposed on the edges of the system (see figure 1). In (c) and (d), edge exchange fields are parallel like (a) and (b), but the exchange fields direction is reversed. In (e) and (f), edge exchange fields are anti-parallel and graphs for spin up and spin down are totallycoincident.

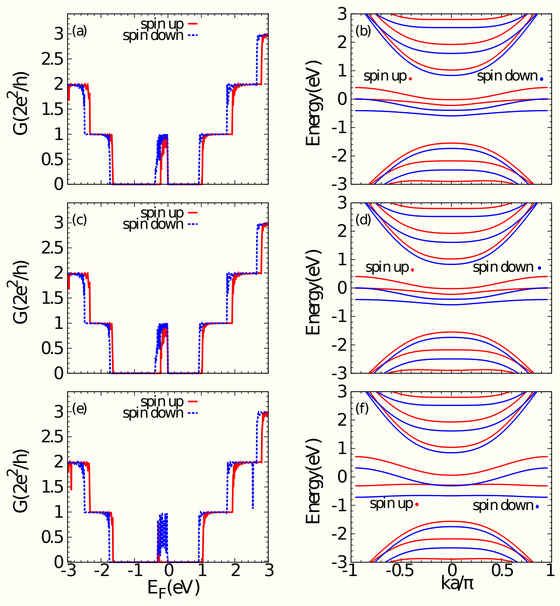


Figure 6: Spin dependent conductance for both spin up and spin down (the left column) and their band structure counterparts (the right column) in the presence of parallel edge exchange fields and different external perpendicular electric fields (E_z). In the first two rows (a)-(d), the electric field strengths are the same but their directions are opposite [i.e., $eE_z = 0.2\,eV/\AA$ in (a) and (b) and $eE_z = -0.2\,eV/\AA$ in (c) and (d)]. In (e) and (f) the electric field magnitude is $eE_z = 0.5\,eV/\AA$.

Conclusions

- In the vicinity of the zero Fermi energy, i.e., $-0.38\,eV < E_F < 0$, there exist two narrow twofold degenerate bands due to the edge states, which play crucial roles in quantum transport properties of $ZPNRs$.
- In the absence of external electric and exchange fields, Near the zero Fermi energy, the degeneracies of two degenerate bands are reduced in the close vicinity of the zero Fermi energy ($-0.23\,eV < E_F < 0$). This band splitting causes the conductance increases in this region.
- For anti-parallel configuration, in the presence of a perpendicular electric field, an spin filtering property occurs in the vicinity of the zero Fermi energy which is raised due to the edge bands of $ZPNRs$. The type of this spin filtering may be changed easily by inversion of the electric field direction.
- For a parallel configuration, edge bands cause spin filtering both in the absence and in the presence of external electric field. This spin filtering is invariant against the reversing of the electric field direction.
- Differences between parallel and anti-parallel configurations originate from the order of the edge bands near the zero Fermi energy. In the former, these bands configure in such a way that two intra adjacent bands have different spin types while in the later one, these two bands have the same spin.
- These properties nominate the $ZPNR$ as a felicitous candidate both for spin filtering devices and spin field effect transistors.

References

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Contacts and Tools

Prof. Dr. Mahdi Esmaeilzadeh
Email: mahdi@iust.ac.ir
Home page: Esmaeilzadeh.iust.ac.ir

Mohammad Ali Mohammadi Keshtan
Email: m_ali_m_keshtan@physics.iust.ac.ir

Tools:
System: Dell Inspiron 5010n series, Corei5 laptop
Operating System : Ubuntu 14.04
Programming: Fortran (double precision), GFortran
Writing : LaTeX
Plotting and picture editing : Gnuplot, Inkscape