Spin control in topological semimetals

Yuriko Baba[1, 2, *], **Rafael A. Molina**[2], **Francisco Domínguez-Adame**[1].
[1]GISC, Departamento de Física de Materiales, UCM
[2]Instituto de Estructura de la Materia, IEM-CSIC

Introduction: Topological materials have attracted great interest since they exhibit new fundamental phenomena and hold great promise for far-reaching technological applications. Their hallmark is **quantized response functions** and the existence of protected gapless surface states named **Fermi arcs**. The gapped case was the first under study, starting the fruitful field of topological insulators. On the other hand, gapless systems assemble the family of topological semimetals. In Dirac and Weyl semimetals the phenomenology is enriched by the **chirality** as a new degree of freedom of the topological states.

Objectives: The objective of this thesis is to study the robustness of the protected topological states as well as to propose mechanisms to control the spin-chiral degree of freedom. In particular we study the effect of:
- Electric fields in the direction of decay of the states
- Rashba spin-orbit coupling induced by local fields in the substrate
- Electric and magnetic fields in Hall bars
- Effects of disorder

Main results:
- The electric field generates a spin-dependent renormalizarion of the Fermi velocity
- The Rashba coupling induces a controllable spin-flip effect
- The effect of magnetic and electric fields create Weyl orbits and induces a Quantum Hall state even in 3D materials

Models for Dirac and Weyl semimetals

- The semimetals can be described by low-energy one-particle Hamiltonians, with parameters obtained from DFT. Each chiral sector is described by:

$$\mathcal{H}_\zeta(\mathbf{k}) = \epsilon_0(\mathbf{k})\mathbb{1}_2 + M(\mathbf{k})\sigma_z + v(\zeta k_x\sigma_x - k_y\sigma_y)\ ,$$

with $\epsilon_0(\mathbf{k}) = c_0 + c_1k_z^2 + c_2(k_x^2+k_y^2)$, $M(\mathbf{k}) = m_0 - m_1k_z^2 - m_2(k_x^2+k_y^2)$, $\zeta = \pm 1$.

- Experimentally realized in materials such as TaAs (Weyl) or Na_3Bi and Cd_3As_2 (Dirac).

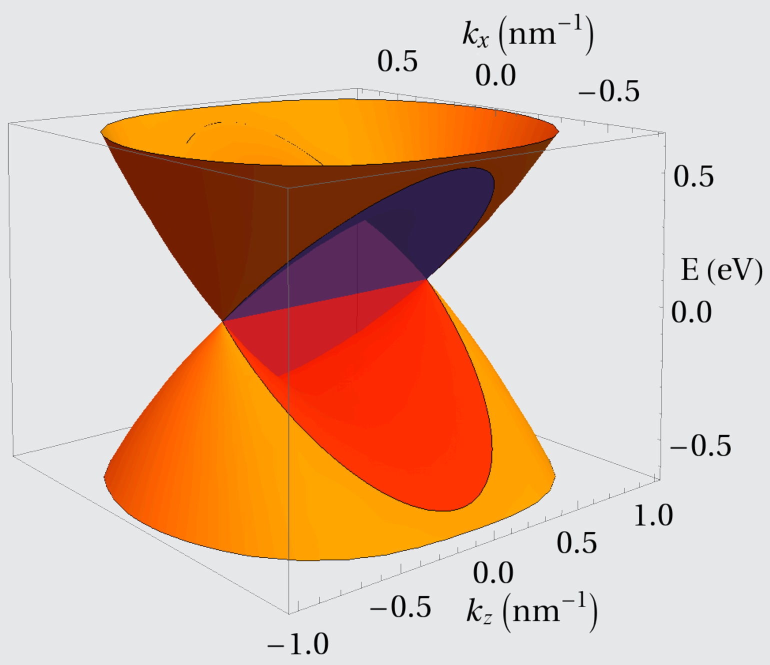
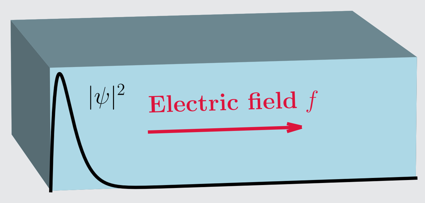


Fig. 1: Particle-hole symmetric spectrum: bulk (orange) and surface (red/blue) bands.

Ingredients for a minimal Weyl/Dirac semimetal:
- at least two nodes;
- four (two) bands for a Dirac (Weyl) semimetal;
- the Chern number of the bands changes with k_z.

Characteristics:
- surface states between the nodes with linearly dispersive bands;
- chiral nodes ⇒ surface states with defined chirality ζ and spin.

Electric field perpedicular to surface



- Electric field perpendicular to the surface, in the direction of decay of the states.
- The bands are displaced and the Dirac cones modified ⇒ **the Fermi velocity changes depending on the chirality**.

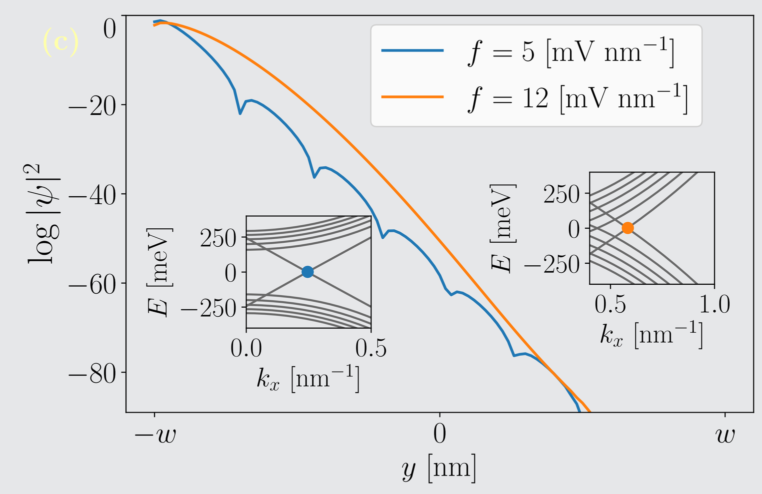


Fig. 2: Type transition induced by the electric field: the surface states change the decay from oscillatory to purely exponential.

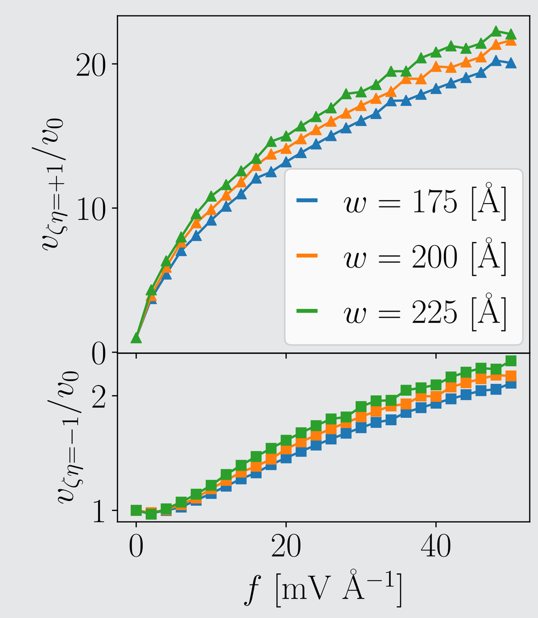


Fig. 3: Chiral-dependent renormalization of the Fermi velocity in a Na_3Bi slab.

Rashba spin-orbit coupling

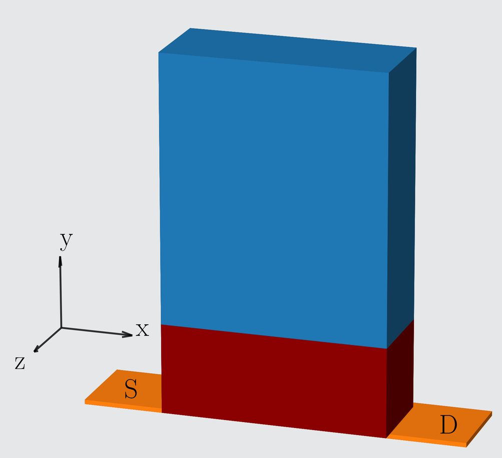
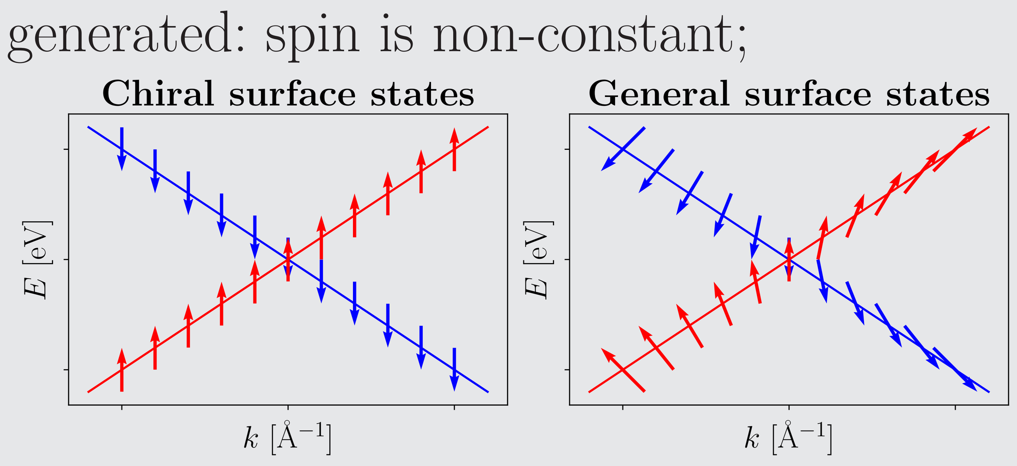


Fig. 4: Set-up: 2 terminals with metallic, spin-polarized and bidimensional leads.

- Coupling between electronic bands due to the breaking of the axial symmetry;
- a more complex spin structure is generated: spin is non-constant;



- **spin-flip conductance** in particle-hole asymmetric bands;
- robustness to disorder.

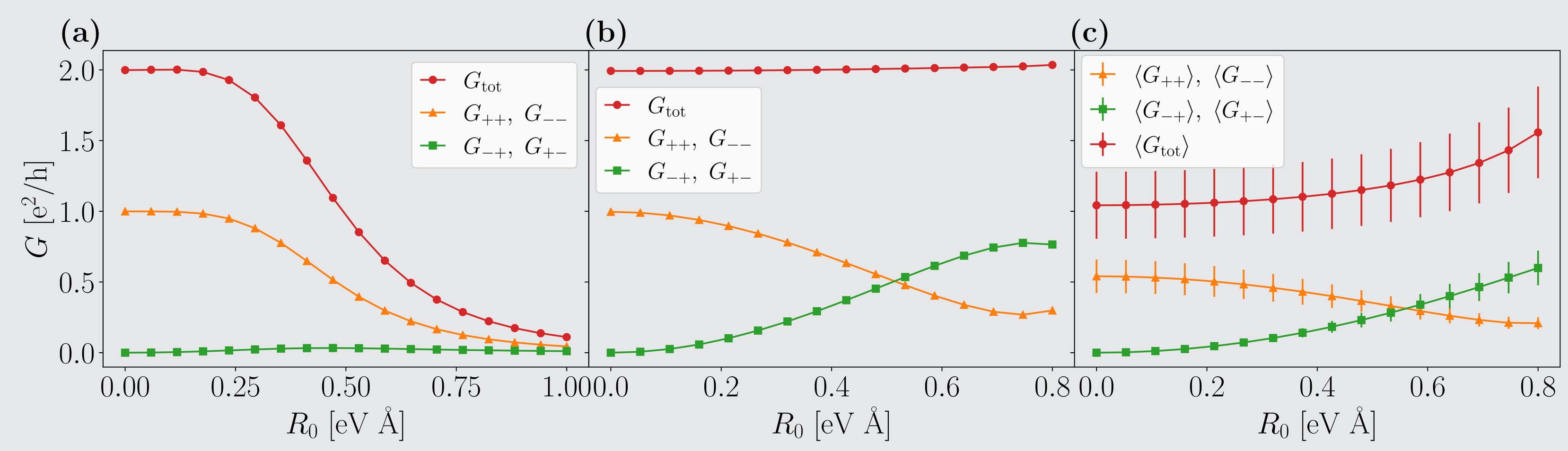


Fig. 5: Total conductance $G_{\rm tot}$ and polarised spin conductances $G_{\pm\pm}$, $G_{\pm\mp}$ as a function of R_0 (Rashba strength) in a Na_3Bi slab with dimensions $150\times150\times100$ Å^3 and $L_{\rm RSOC} = 50$ Å. **(a)** particle-hole scenario, **(b)** pristine Na_3Bi slab, **(c)** average conductance in the presence of point-like impurities with density $n_{\rm imp} = 4\cdot10^{19}{\rm cm}^3$.

Current research

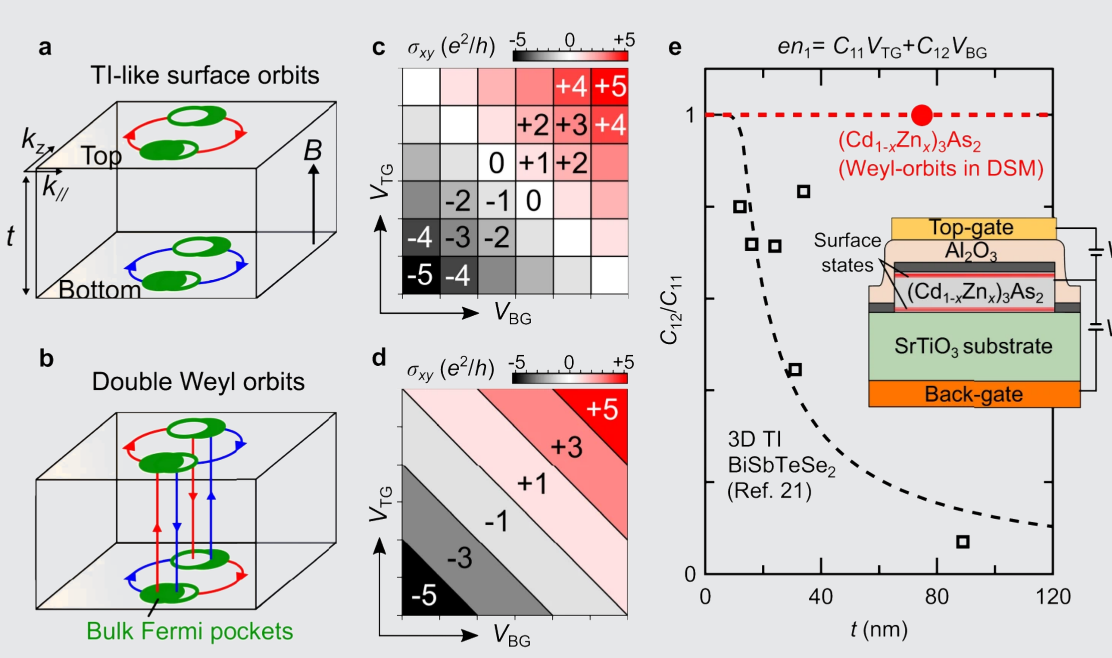


Fig. 6: Experimental proposal of *Nature Communications* **12**, 2572 (2021)

- Effect of both electric and magnetic field to induce Weyl orbits and Quantum Hall states in 3D;
- inclusion of disorder and impurities;
- simulation of more realistic set-ups: Hall bars and multi-terminal.

References

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* yuribaba@ucm.es
@yurikoBD
@qng_ucm