Conductance of Edge Modes in Nanoribbons of 2D Materials in a Topological Phase

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***Abstract*—Employing novel 2D materials with topologically protected current-carrying states is promising to boost the on-current. Based on an effective k·p model, we analyze the topologically protected states and their conductance for several 2D materials. We compare the 2D materials MoS_2, WS_2, and WSe_2 and find the largest electric field-induced conductance modulation in 1T′ MoS_2 nanoribbons.**

Keywords- topologically protected edge states; topological insulators; nanoribbons; k·p method, conductance

I. INTRODUCTION

The use of novel materials with advanced properties is mandatory to continue with device scaling for high performance applications at reduced power. Topological insulators (TIs) belong to a new class of materials possessing highly conductive edge states with a nearly linear dispersion lying in the band gap of the TI. These states are topologically protected and, therefore, immune to backscattering from defects and disorder. Well-known monolayer-thin two-dimensional (2D) materials can also be in a TI phase [1]. The fundamental band gap within which the edge states lie decreases with the perpendicular electric field E_z created by the gate voltage and closes at some critical field. The gap re-opens at higher E_z, however the TI becomes a normal semiconductor with no edge states, and the on-current is switched off [1].

To enhance the on-current due to the edge states it is mandatory to have many edges by stacking several nanoribbons. In this work we evaluate the edge states and their corresponding Landauer conductance in a nanoribbon in the 1T′ TI phase. The 2D materials considered are MoS_2, WS_2, and WSe_2.

II. Method

The effective Hamiltonian $H(k)$ inside the nanoribbon of the width d is [2]:

$$H(k) = \begin{pmatrix} \frac{1}{2} - k_y^2 \frac{m}{m_y^p} - k_x^2 \frac{m}{m_x^p} & v_2 k_y - \alpha E_z + i v_1 k_x \\ v_2 k_y - \alpha E_z - i v_1 k_x & \frac{-1}{2} + k_y^2 \frac{m}{m_y^d} + k_x^2 \frac{m}{m_x^d} \end{pmatrix}$$

Here energies are measured in units of the gap δ occurring at the Γ-point of the inverted band structure , the wave vectors $k = (k_x, k_y)$ is in units $k_0 = \sqrt{\frac{2\delta}{\hbar^2} \frac{m_y^d m_y^p}{m_y^d + m_y^p}}$, where $m_{y(x)}^{d(p)}$ are the effective masses, $m = \frac{m_y^d m_y^p}{m_y^d + m_y^p}$ and $v_{1(2)}$ are the dimensionless velocities. The nanoribbon is cleaved along the *OX* axes so that the wave function in the quantization *OY* direction satisfies $\psi_{k_x}(\pm d/2) = 0$. The wave functions and the edge modes dispersion relations are found numerically using the Newton method [3]. The conductance of the modes is then evaluated as a function of the effective electric field E_z, for several nanoribbon widths made of the aforementioend 2D materials.

III. RESULTS

Fig.1 shows the subband structure in a 20nm wide 1T'-MoS_2 nanoribbon at $E_z = 0$. The subbands with a nearly linear dispersion correspond to the edge modes. A small gap opens in the linear spectrum at $k_x = 0$ due to the interaction of modes localized at the opposite edges. Fig.2 shows the dependence of the bottom of the electron-like and the top of the hole-like edge modes energies as a function E_z, for several widths. As expected, the gap between them shown in Fig.3 increases if the width of the nanoribbon decreases. In contrast to the separation of the electron and hole extrema in the bulk (shown with dashed lines in Fig.2), the gap between the edge modes also increases as a function of the electric field E_z as shown in Fig.3.

Because the energy gap between the edge modes grows with E_z, the corresponding Landauer conductance drops. Fig.4-6 show the conductance behavior as a function of E_z for several widths, for MoS_2, WS_2, and WSe_2 nanoribbons. The decrease of the conductance is non-universal and depends strongly on the material as well as on the nanoribbon width. The decrease is only a few percent in WSe_2 and about 10% in WS_2. At room temperature the largest conductance modulation by the electric field of about 20% is found for 1T′ MoS_2 nanoribbons. The modulation is expected to increase significantly, at least by an order of magnitude [4], if the scattering between the modes is taken into account at larger E_z when the bulk material becomes a normal semiconductor.

IV. CONCLUSION

A **k·p** method is applied to investigate the topologically protected states at the edges of nanoribbons of several 2D materials. It is demonstrated that the perpendicular electric field-induced conductance modulation is the largest in 1T′ MoS_2 nanoribbons making them more suitable candidates for use in ultra-scaled devices.

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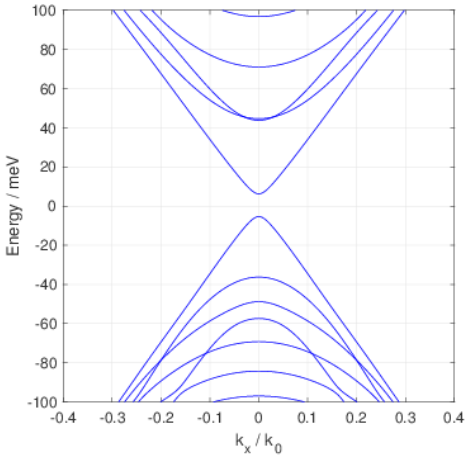

Fig.1: *Subband structure in a MoS_2 nanoribbon with width d=20nm at $E_z = 0$. The subbands with the linear dispersion and a small gap at $k_x = 0$ correspond to the edge modes.*

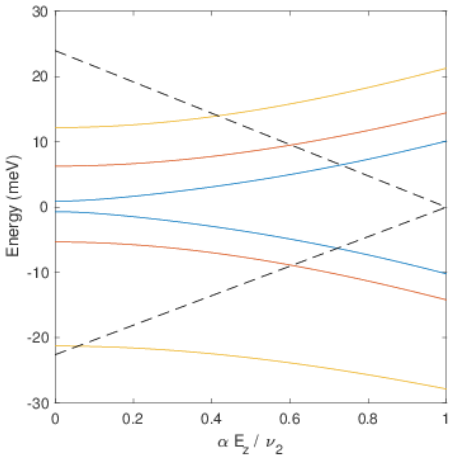

Fig.2: *Energies of the electron and hole edge states in a MoS_2 nanoribbon of the width d=30nm (blue), d=20nm (orange) and d=10nm (yellow) as a function of electric field strength. Dashed line: bulk bands extrema.*

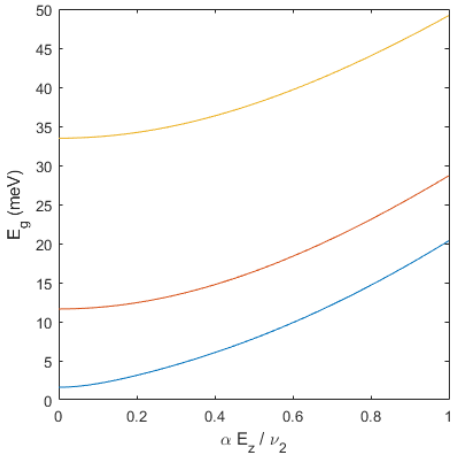

Fig.3: *Energy gap in the edge states spectrum in a MoS_2 nanoribbon of the width d=30nm (blue), d=20nm (orange) and d=10nm (yellow) as a function of electric field strength.*

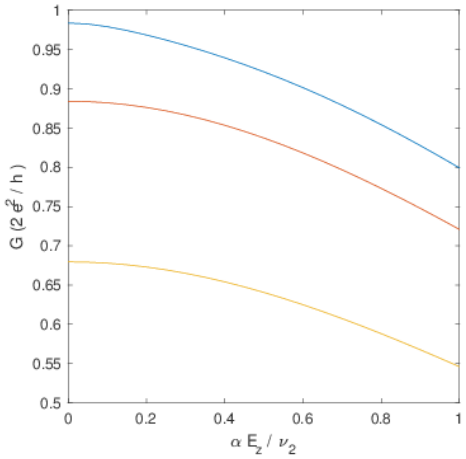

Fig.4: *Ballistic conductance as a function of electric field strength due to the lowest electron and topmost hole edge states for a MoS_2 nanoribbon of the width d=30nm (blue), d=20nm (orange) and d=10nm (yellow).*

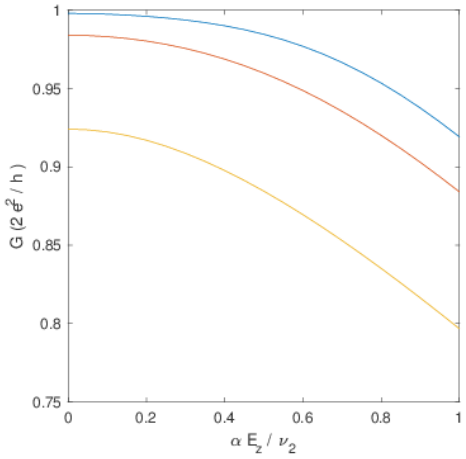

Fig.5: *Ballistic conductance as a function of electric field strength due to the lowest electron and topmost hole edge states for a WSe_2 nanoribbon of the width d=30nm (blue), d=20nm (orange) and d=10nm (yellow).*

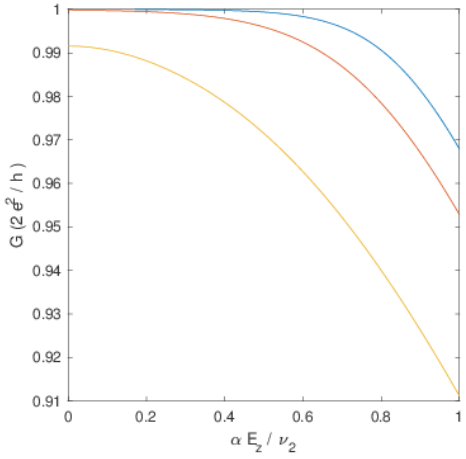

Fig.6: *Ballistic conductance as a function of electric field strength due to the lowest electron and topmost hole edge states for a WS_2 nanoribbon of the width d=30nm (blue), d=20nm (orange) and d=10nm (yellow).*