

# Ballistic conductance in a topological 1T' MoS<sub>2</sub> Nanoribbon

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**Abstract.** A MoS<sub>2</sub> sheet in its 1T' phase is a two-dimensional topological insulator. It possess highly conductive edge states which due to topological protection, are insensitive to back scattering and are suitable for device channels. A transition between the topological and conventional insulator phases in a wide 1T'-MoS<sub>2</sub> sheet is controlled by an electric field orthogonal to the sheet. In order to enhance the current through the channel several narrow nanoribbons are stacked. We evaluate the subbands in a narrow nanoribbon of 1T'-MoS<sub>2</sub> by using an effective **k**·**p** Hamiltonian. In contrast to a wide channel, a small gap in the spectrum of edge states in a nanoribbon increases with the electric field. It results in a rapid decrease in the nanoribbon conductance with the field, making it potentially suitable for switching.

Edge states in two-dimensional (2D) topological insulators (TI) propagate without backscattering, making them attractive for designing highly conductive transistor channels [1]. However, possessing robust conductive channels is only one requirement for a good transistor. To make a switch it is necessary to suppress the current through the channel as a function of gate voltage. A standard approach is to restore the traditional band order [2]. Recently it was discovered that the 1T' phase of MoS<sub>2</sub>, a well-known 2D material with a high promise for future microelectronic devices [3], is a TI [4]. The inverted band structure is well approximated by parabolas, with the conduction and valence bands having masses of  $m_{y(x)}^{d(p)}$  [4]. The spin-orbit interaction opens a gap at the intersection of the valence and conduction bands, which appears at a finite value of the momentum  $k_y$  along the quantization axis *OY* (Fig. 1, solid green lines). A topologically protected highly conductive edge state must exist within the gap. By applying an electric field  $E_z$  along the *OZ* axis perpendicular to the nanoribbon the gap at one of the minima can be reduced, closed (Fig. 1, dotted red lines), and open again (Fig. 1, dashed-dotted blue lines) at large electric fields. The gap at large electric fields becomes a direct gap, so no edge states are allowed within the bulk gap. In order to investigate transport through a nanoribbon, the subband structure and the wave functions must be evaluated first. We parametrize the energy in units of the band inversion gap  $2\delta$  at  $k_y = 0$ , while  $k_{y(x)}$  in units of  $k_0 = \left(\frac{2\delta}{\hbar^2} \frac{m_y^d m_y^p}{m_y^d + m_y^p}\right)^{1/2}$ . By applying a unitary transformation, the  $4 \times 4$  Hamiltonian [4] is cast in a block-diagonal form [5]:

$$\mathbf{H} = \begin{pmatrix} H(\mathbf{k}) & 0 \\ 0 & H^*(-\mathbf{k}) \end{pmatrix}. \quad (1)$$

The possibility to express the Hamiltonian in the form (1) is a consequence of the time-reversal symmetry [5]. It then follows that at every edge, if allowed, there are two topologically protected modes propagating in opposite directions with opposite spins. The  $2 \times 2$  Hamiltonian  $H(\mathbf{k})$ ,  $\mathbf{k} = (k_x, k_y)$  in dimensionless units has the form:

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

$m = \frac{m_y^d m_y^p}{m_y^d + m_y^p}$  and  $v_{1(2)}$  are the Fermi-velocities. We consider a nanoribbon with a width in the *OY* direction of  $d =$

$40k_0^{-1} \approx 27$  nm. A subband wave function,  $\psi_{k_x}(y) = \sum_{j=1}^4 A_j \exp'(ik_j y)$ , where  $A_j$  is a two-component spinor, is set to zero at both edges. The dispersion equation is solved numerically, in complete analogy to the problem of finding the eigenenergies and eigenfunctions for a 2-band **k**·**p** Hamiltonian in silicon films [6]. Figs 2,3, and 4 show the dispersion for several electron and hole subbands. A peculiar feature, which distinguishes the subband structure from that in silicon films, is the presence of the subband with nearly linear dispersion (Fig. 2). The energy of the subband lies in the band gap seen in Fig. 1. The solution corresponds to the topologically protected edge modes. A small gap is opened at  $k_x = 0$  reflecting the fact that the topological states located at the two opposite edges interact. By increasing  $E_z$  the gap between the subbands electron (hole) subbands minima (maxima)  $E_i^{e(h)}$  grows (Fig. 5). It exists (Fig. 3) even when the gap in the bulk is zero (Fig.1, dashed red). The behavior is in sharp contrast to that in a wide ribbon. The nanoribbon ballistic conductance

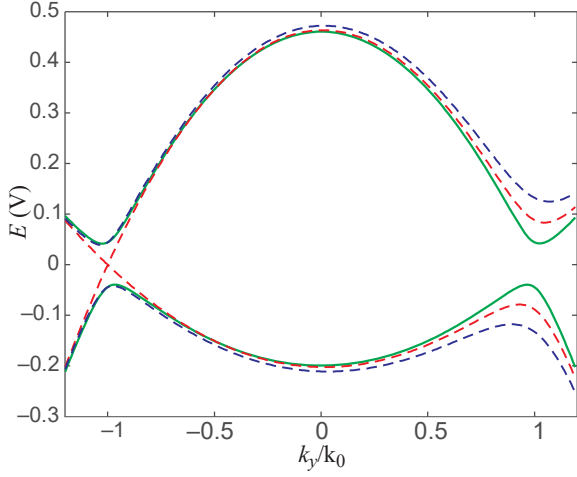
$$G = \frac{2e^2}{h} \sum_i \left[ \frac{1}{1 + \exp \frac{E_i^e - E_F}{k_B T}} + \frac{1}{1 + \exp \frac{E_F - E_i^h}{k_B T}} \right] \quad (3)$$

as a function of  $E_z$  is shown in Fig.6. Due to the growing gap (Fig.5),  $G$  decreases rapidly with the field. This makes 1T'-MoS<sub>2</sub> potentially suitable for transistor applications.

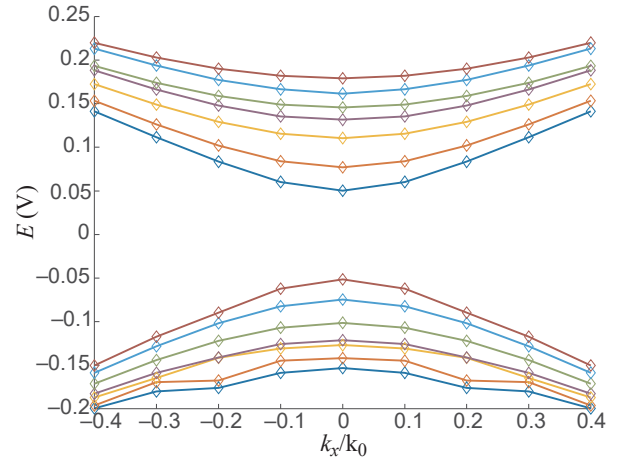
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## References

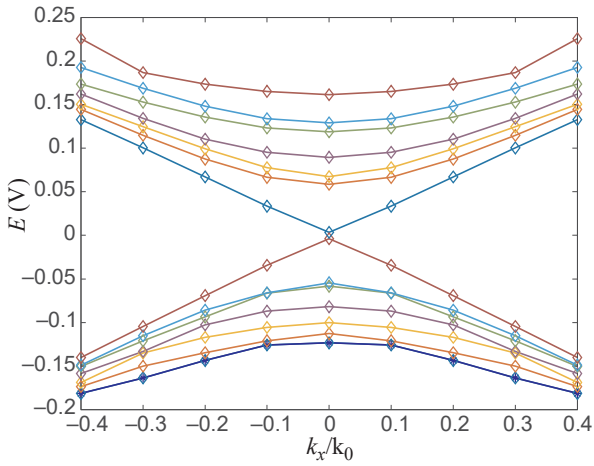
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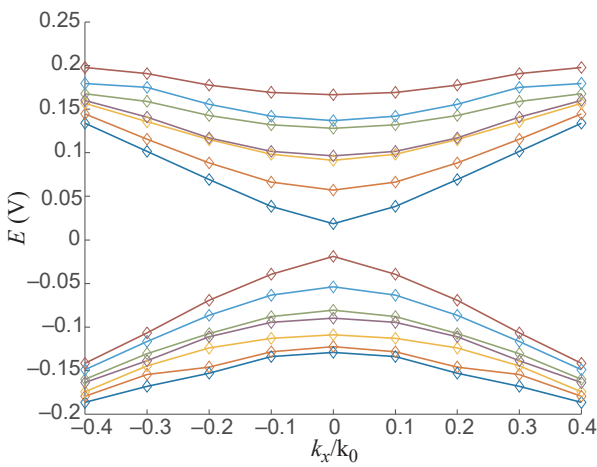
**Fig. 1.** Bulk bands in 1T'-MoS<sub>2</sub> with an inverted gap at  $k_y = -k_0$  at  $E_z = 0$  (solid lines), the gap closed at  $\alpha E_z = \hbar k_0 v_2$  (dashed lines) and open as a direct gap at  $(\alpha E_z = 2\hbar k_0 v_2)$ , dashed-dotted lines).



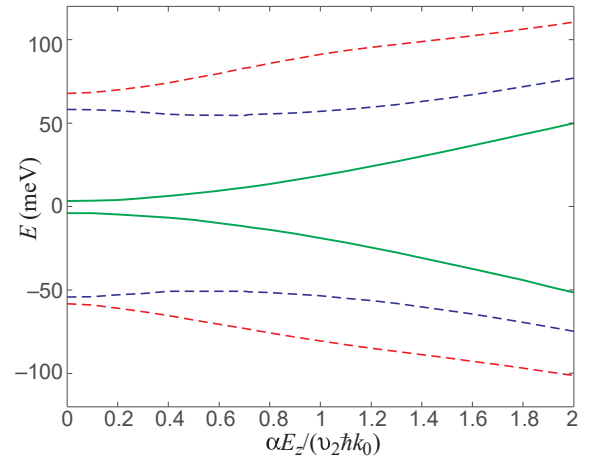
**Fig. 4.** Subband energies in a nanoribbon of the width  $d = 40/k_0$  at  $\alpha E_z = 2\hbar k_0 v_2$ , when the direct gap opens again at  $k_y = -k_0$ , see Fig.1, dashed-dotted lines.



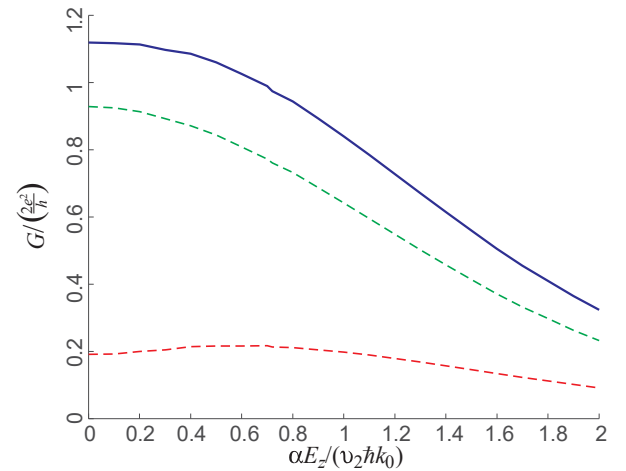
**Fig. 2.** Subbands in a nanoribbon of the width  $d = 40/k_0$  at  $E_z = 0$ . The subband with an almost linear dispersion corresponding to the topologically protected edge state is clearly seen.



**Fig. 3.** Subband energies in a nanoribbon of the width  $d = 40/k_0$  at  $\alpha E_z = \hbar k_0 v_2$ , when the gap at  $k_y = -k_0$  is closed, see Fig.1, dashed lines.



**Fig. 5.** Dependence of electron (hole) subbands minima (maxima) on the electric field  $E_z$ . In contrast to the bulk case, the gap never closes and keeps increasing with  $E_z$  growing.



**Fig. 6.** Ballistic conductance (solid line) of a 1T'-MoS<sub>2</sub> nanoribbon, with the contributions due to the first edge-like states (dashed line), and bulk-like subbands (dashed-dotted line).