Topologically Protected and Conventional Subbands in a 1T'-MoS_2 Nanoribbon Channel

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***Abstract*—Continuous miniaturization brought the silicon technology to the nanometer scale where performance enhancement cannot be easily achieved by further feature size reduction. The use of new material with advanced properties has become mandatory to meet the needs for higher performance at reduced power. Topological insulators possess highly conductive topologically protected edge states insensitive to scattering and thus suitable for energy efficient high speed devices. Here, we evaluate the subband structure in a nanoribbon of 1T'-MoS_2 by applying an effective k.p Hamiltonian in a confined geometry.**

Keywords - Topological insulators, topologically protected edge states, nanoribbons, subbands, k.p Hamiltonian

Topological insulators (TIs) belong to a new class of semiconducting materials with highly conductive surface states. Recent progress in fabrication and investigation of two-dimensional (2D) TIs [9] demonstrates the potential of these materials for further use in microelectronics. These edge states lie in the band gap of the bulk insulating material. In order to allow the states within the gap, the bulk host material must possess an inverted band structure with the valence band edge lying above the conduction band edge. The standard band order is restored at the edge where the host material is interfaced with a normal dielectric (air). The edge states then possess a linear Dirac-like energy dispersion. The edge states in 2D TIs are topologically protected by time-reversal symmetry, which results in electron propagation without backscattering. This property makes them attractive as a material for high conductive transistor channels.

Having highly robust conductive channels is not sufficient to make a good transistor switch as one has to have a possibility to suppress the current through the channels. A plausible option is to close the gap in the host bulk material. In this case scattering between the protected edge and the non-protected electron-hole bulk states results in strong scattering, which effectively reduces the current through the edge states [2]. In the case when the normal gap in the bulk material is created by restoring the order of the bands, there are no edge states allowed within the gap, and the current is stopped completely.

Recently it was discovered that if the well-known 2D material MoS_2 which has a high promise for future microelectronic devices [3] is grown in a 1T' phase, it becomes a TI [4]. The inverted band structure is well described by the parabolic conduction and valence bands with the masses $m_{y(x)}^{d(p)}$ [4].

Without spin-orbit interaction included, the material is a semi-metal. 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 perpendicular to the nanoribbon (Fig.1, green). In the nanoribbon topologically protected highly conductive edge states 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, red), or even open again (Fig.1, blue) 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 and scattering 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 2δ at k_y=0, while $k_{y(x)}$ in units of $k_0 = \left(2\frac{\delta}{\hbar^2}\frac{m_y^d m_y^p}{m_y^d+m_y^p}\right)^{1/2}$ to write the 4x4 k.p Hamiltonian H [4] in dimensionless units. By applying a unitary transformation, the Hamiltonian H is re-written in a block-diagonal form [5]

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

The possibility to express the Hamiltonian in the form (1) is a consequence of the time-reversal symmetry. It then follows that, if allowed, at every edge there are two topologically protected modes propagating in opposite directions with opposite spins. The 2x2 Hamiltonian $H(\mathbf{k}), \mathbf{k} = (k_x, k_y)$ in dimensionless units has the form:

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

where $m = \frac{m_y^d m_y^p}{m_y^d+m_y^p}$ and $v_{1(2)}$ are the dimensionless Fermi-velocities.

Let us consider a nanoribbon with the width in OY direction d=40/k_0. To evaluate the subband structure, we look for the solution $\psi_{k_x}(y) = \sum_{j=1}^{4} A_i \exp(ik_j y)$, where A_i is a two-component constant spinor. We obtain the subbands eigenenergies and wave functions by setting the wave function to zero at both edges. The dispersion equation is solved numerically, in a complete analogy to the problem of finding the eigenenergies and eigenfunctions for a 2-band k.p Hamiltonian in silicon films [6].

Fig.2 displays the subband energies as a function of k_x, for several lowest subbands. The peculiar feature which distinguishes the subband structure from that in silicon films is the presence of the subband with a nearly linear dispersion. The energy of the subband is lying within the bulk band gap (Fig.1). This solution corresponds to the topologically protected edge mode,

which is confirmed by the complex values of the solutions for k_j . A close inspection demonstrates that a very small gap is opened at $k_x = 0$ reflecting the fact that the topological states located at the two opposite edges of the nanoribbon are not independently propagating and start interaction at small k_x. At larger k_x the coupling between the edge states becomes insignificant as the edge states are moving in opposite direction.

The gap between the bulk bands is altered by the out-of-nanoribbon electric field E_z. By increasing E_z the gap can be reduced, closed, and open again as a direct gap at one of the minima, Fig.1. This leads to the gap between the lowest subbands opening (Figs 3,4), and the linear dispersion becomes more quadratic close to the subband minimum. At the same time the edge mode delocalises from the edge as two of k_j become real, which leads to increased scattering and results in a reduced current.

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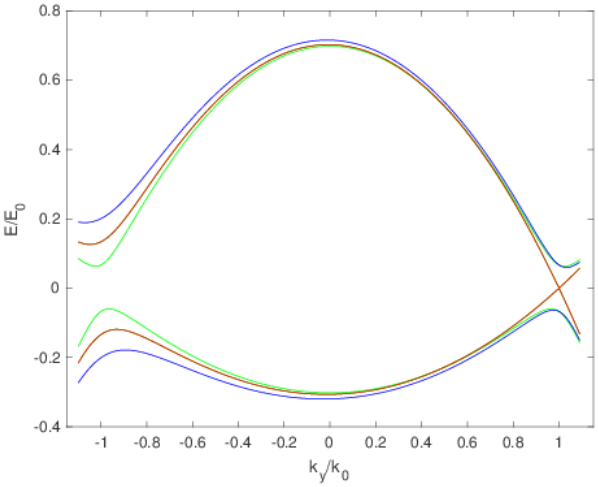

Fig.1. Bulk energy dispersion in 1T'-MoS_2 two-dimensional material. Green dispersion displays the gaps at k_y=k_0 in the inverted band structure at E_z=0. Increasing the electric field to E_z=-v_2 closes the gap (red curve) and reopens it again as a direct gap (E_z=-2v_2 , blue curve).

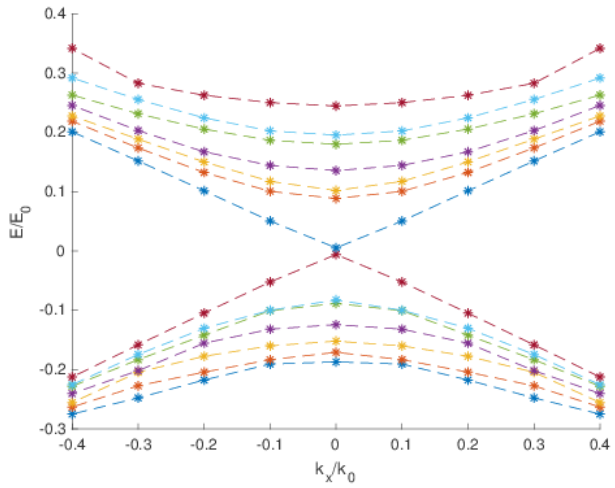

Fig.2. Subbands in a nanoribbon of the width d=40/k_0. E_z=0. The subband with an almost linear dispersion corresponding to the topologically protected edge state is clearly seen.

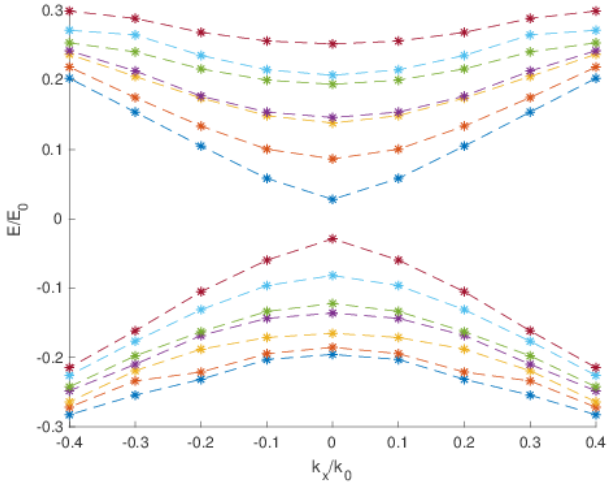

Fig.3. Subband energies at E_z=-v_2, when the gap at k_y=k_0 is closed, see Fig.1, red curve.

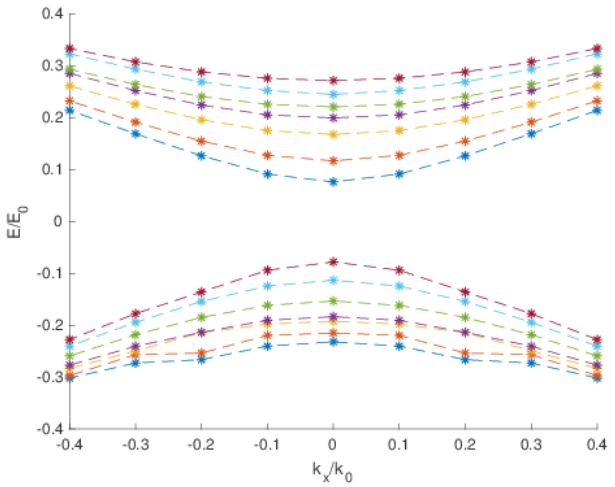

Fig.4. Subband energies at E_z=-2v_2, when the gap at k_y=k_0 is closed, see Fig.1, blue curve.