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SPIN RELATED PHENOMENA IN NANOSTRUCTURES

Ballistic Conductance in a Topological $1T'$-MoS_2 Nanoribbon

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Abstract—A MoS_2 sheet in its $1T'$ phase is a two-dimensional topological insulator. It possesses 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_2 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_2 by using an effective $\mathbf{k} \cdot \mathbf{p}$ 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 current switching.

Keywords: topological insulators, topologically protected edge states, nanoribbons, subbands, $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian, ballistic conductance

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1. INTRODUCTION

Edge states in two-dimensional (2D) topological insulators (TI) propagate without backscattering, which makes 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_2, 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). 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), and open again (Fig. 1, dotted–dashed blue) at large electric fields. The gap becomes a direct gap, so no edge states are allowed within the bulk gap.

2. METHODS

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 2δ at $k_y = 0$, while $k_{y(x)}$ in units of $k_0 = \left(2\frac{\delta}{\hbar^2}\frac{m_y^d m_y^p}{m_y^d + m_y^p}\right)^{1/2}$. By applying a unitary transformation, the 4×4 Hamiltonian [4] is cast in a block-diagonal form [5].

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

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 propagat-

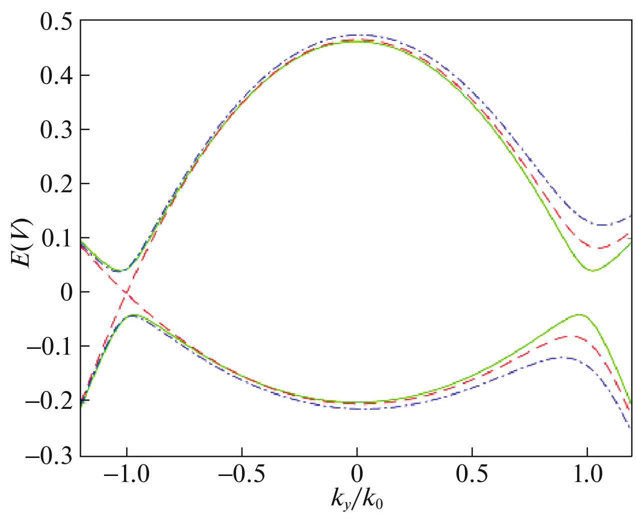

Fig. 1. Bulk energy dispersion in $1T'$-MoS_2 2D material. The solid green lines display the gaps at $k_y = k_0$ in the inverted band structure at $E_z = 0$. Increasing the electric field to $\alpha E_z = \hbar k_0 v_2$ closes the gap (dashed red lines) and reopens it again as a direct gap ($\alpha E_z = 2\hbar k_0 v_2$, dotted-dashed blue lines).

ing in opposite directions with opposite spins. The 2 × 2 Hamiltonian $H(\mathbf{k})$, $\mathbf{k} = (k_x, k_y)$ in dimensionless units has the form:

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

$m = \dfrac{m_y^d m_y^p}{m_y^d + m_y^p}$ and $v_{1(2)}$ are the velocities.

We consider a nanoribbon with a width in the *OY* direction of $d = 40/k_0 \approx 27$ nm. A subband wave function, $\psi_{k_x}(y) = \sum_{j=1}^{4} A_j \exp(ik_j y)$, where A_i 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 $k \cdot p$ Hamiltonian in silicon films [6].

3. RESULTS AND DISCUSSION

Figure 2 shows 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. 2a). 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. 3a). It exists (Fig. 2b) 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

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

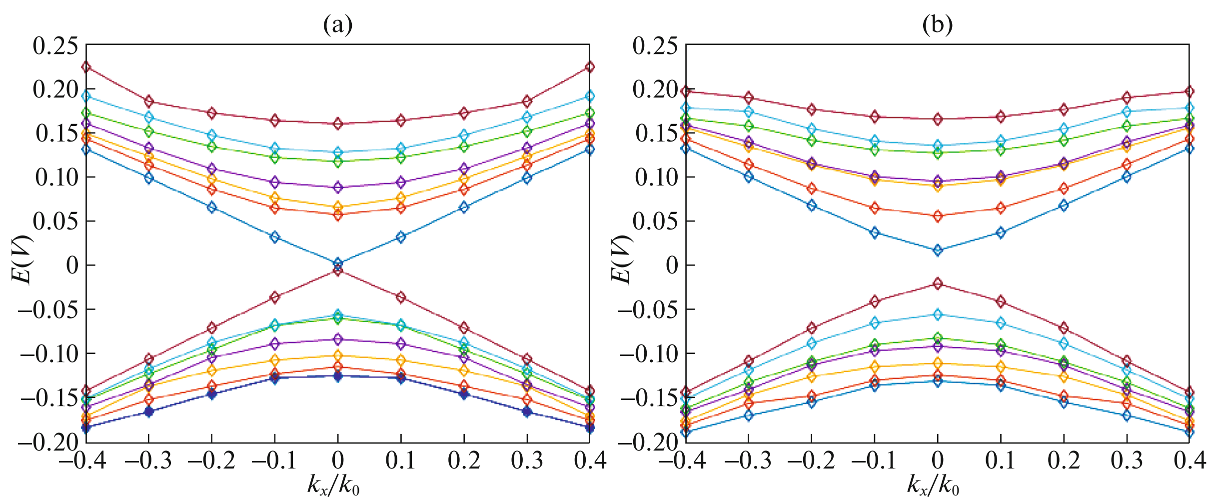

Fig. 2. Subbands in a nanoribbon of width $d = 40/k_0$: (a) $\alpha E_z = 0$. The subband with an almost linear dispersion corresponding to the topologically protected edge state is clearly seen; (b) Subband energies at $\alpha E_z = \hbar k_0 v_2$, when the gap at $k_y = k_0$ is closed, see Fig. 1, dashed red lines.

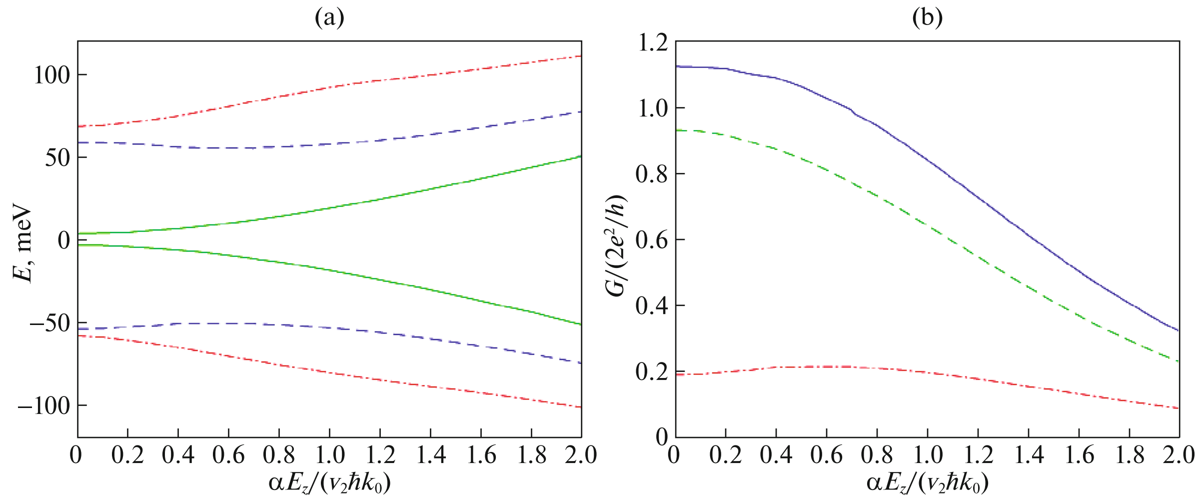

Fig. 3. (a) Dependence of electron (hole) subband minima (maxima) on the electric field E_z for the first three subbands. In contrast to the bulk case, the gap never closes and keeps increasing with E_z growing a nanoribbon of the width $d = 40/k_0$. (b) Ballistic conductance (solid blue) of a $1T'$-MoS_2 nanoribbon, with the contributions due to the first edge-like states (dashed green line), and the remaining bulk-like subbands (dotted-dashed red line).

as a function of E_z is shown in Fig. 3b. Due to the growing gap (Fig. 3a), the conductance G decreases rapidly with the field. This makes $1T'$-MoS_2 potentially suitable for transistor applications.

4. CONCLUSIONS

The subband structure in a narrow nanoribbon of $1T'$ molybdenum disulfide as a function out-of-plane electric field is evaluated by employing the effective four-band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. In contrast to the behavior at an edge of a two-dimensional sheet, where the bulk gap closes at a certain field value, the gap between the traditional lowest electron and highest hole subband never closes in a nanoribbon. Instead, it increases with the perpendicular electric field.

A tiny gap in the spectrum of the edge states opened in a nanoribbon increases rapidly with the perpendicular electric field. It results in a substantial decrease of the ballistic conductance. Thus, varying the electric field is attractive for designing MoS_2 nanoribbon-based current switches.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interest related to this work.

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