Subband Structure and Ballistic Conductance of a Molybdenum Disulfide Nanoribbon in Topological 1T' Phase: A k∙p Study

Viktor Sverdlov
Christian Doppler Laboratory for Nonvolatile Magnetoresistive Memory and Logic at the Institute for Microelectronics Technische Universität Wien Vienna, Austria sverdlov@iue.tuwien.ac.at

Al-Moatasem Bellah El-Sayed, Siegfried Selberherr Institute for Microelectronics Technische Universität Wien Vienna, Austria al-sayed@iue.tuwien.ac.at, Selberherr@TUWien.ac.at

Abstract—We evaluate the subband structure in a narrow nanoribbon of 1T' molybdenum disulfide by employing an effective k∙p Hamiltonian. Highly conductive topologically protected edge states whose energies lie within the bulk band gap are investigated. Due to the interaction of the edge modes located at the opposite edges, a small gap in their linear spectrum opens in a narrow nanoribbon. This gap is shown to sharply increase with the perpendicular out-of-plane electric field, in contrast to the behavior in a wide nanoribbon. The gaps between the electron and hole bulk subbands also increase with the electric field. The increase of the gaps between the subbands leads to a rapid decrease of the ballistic nanoribbon conductance and current with the gate voltage, which can be used for designing molybdenum disulfide nanoribbon-based current switches.

Keywords—topological insulators, topologically protected edge states, nanoribbons, subbands, k.p Hamiltonian, ballistic conductance

I. INTRODUCTION

Edge states in two-dimensional (2D) topological insulators (TI) propagate without backscattering, making them attractive for designing highly conductive channels [1]. Recently it was discovered that the 1T' phase of MoS2, a well-known 2D material with a high promise for future microelectronic devices [2], is a TI [3]. The inverted band structure is well approximated by parabolas, with the conduction and valence bands having masses of m_p^{(p)} [3]. 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_z along the OZ axis. A topologically protected highly conductive edge state with a linear Dirac-like energy dispersion on the momentum k_x parallel to the OX axis must exist within this spin-orbit gap [3].

However, possessing robust conductive channels is only one requirement. To make a good switch it is necessary to suppress the current through the channel as a function of a perpendicular electric field induced by a gate. A standard approach is to close the gap in the bulk host 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 [4].

By applying an electric field E_z along the OZ axis perpendicular to a MoS2 sheet in the 1T' phase, the bulk spin-orbit gap can be reduced, closed, and opened again as a "negative" gap at large electric fields [3]. The traditional band order is restored from the inverted band structure, the gap becomes a direct gap, and no edge states are allowed in the gap. This transition between the topological and conventional insulator phases in a wide 1T'-MoS2 controlled by the electric field orthogonal to the sheet eliminates the edge states completely and can be used to further suppress the current [5]. In order to enhance the current through the channel it is beneficiary to have many edges by stacking several narrow nanoribbons. Here, we evaluate the subband structure in a narrow nanoribbon of 1T'-MoS2 by using an effective k∙p Hamiltonian [3]. In contrast to a wide channel, we find that a small gap in the spectrum of edge states in a nanoribbon [6] increases with the electric field. It results in a rapid decrease in the nanoribbon conductance with the field, which is potentially suitable for switching.

II. METHOD AND RESULTS

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_z=0, while k_{x(1)} in units of k_0 = (4ħ (m_p m_n)^{1/2} / (2Δ)). By applying a unitary transformation [7], the 4×4 Hamiltonian [3] is cast in a block-diagonal form similar to the one in [6].

\[
H(k) = \begin{pmatrix}
0 & H^*(-k)
\end{pmatrix}
\]

The 2×2 Hamiltonian H(k), k=(k_x, k_y) in dimensionless units has the form

\[
H(k) = \begin{pmatrix}
\frac{1}{2} - k_x^2 m_n & -k_y^2 m_n & -v_x k_x & v_y k_y \\
-k_y^2 m_n & \frac{1}{2} + k_x^2 m_n & v_y k_y & -v_x k_x
\end{pmatrix}
\]

(2)

where \( m = \frac{m_p m_n}{m_p + m_n} \) and \( v_{x(2)} \) are the dimensionless velocities. The parameters used in (2) are from [3] and listed in Table I.

The bulk energy dispersion obtained with the Hamiltonian (2) with an offset of \( ΔE = 1/2 \) is shown in Fig. 1 for several \( k_x \) and \( E_z=0 \). The spin-orbit gap opened at \( k_x = ± k_0 \) is increasing with \( k_0 \). Indeed, the gap is determined by the off-diagonal terms in (2). Since the off-diagonal terms in (2) can be written as \( σ_y k_x \) and \( σ_x v_x k_y \), where \( σ_y \) are the Pauli matrices, the gap \( Δ \) is defined by \( Δ = (ν_x^2 k_x^2 + ν_y^2 k_y^2)^{1/2} \).

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By applying an electric field $E_z$ along the OZ axis the gap at one of the minima (Fig. 2, solid line) can be reduced, completely closed (Fig. 2, dashed line), or even be opened again (Fig. 1, dot-dashed line) at large electric fields. The gap at large electric fields becomes direct.

Let us consider a nanoribbon with a width in the OY direction of $d=40/k_0$. Only quantized values of the momentum $k_y$ along the quantization axis OY are allowed. In addition, it is expected that at $E_z=0$ two topologically protected highly conductive edge states localized at opposite interfaces of a nanoribbon exist at any particular energy $E$ within the gap opened by the spin-orbit interaction at $k_y=\pm k_0$.

A general form of the subband wave function $\psi_{k_y}(y)$ in the quantization OY direction is written as

$$\psi_{k_y}(y) = \sum_{j=1}^{4} A_j \left( \frac{1}{a(k_j,E)} \right) \exp(ik_jy),$$

where $k_j$, $j=1,\ldots,4$ are the roots of $E(k_x,k_y)=E$. $A_j$ are constants, and

The subband energies are obtained by setting the wave function to zero at both edges. The characteristic equation

$$\det(M) = 0,$$

where the matrix $M = (M_1 \ M_2 \ M_3 \ M_4)$ is composed of the columns $M_j$, $j=1,\ldots,4$.

is solved numerically, in complete analogy to the problem of finding the eigenenergies and eigenfunctions of a 2-band $k\cdot p$ Hamiltonian in silicon films [8]. Fig. 3 displays the behaviour of the real part (the imaginary part is zero for $E_z=0$) of the determinant as a function of energy, for $k_x=0$. We are interested in the real part of the determinant, which indicates the presence of topological edge states within the gap.

$$M_j = \begin{pmatrix} 1 \\ a(k_j,E) \exp(ik_jy) \\ a(k_j,E) \exp(ik_jd) \\ \alpha(k_j,E) \end{pmatrix},$$

Table 1 summarizes the parameters used in the model.

### Table 1: Parameters Used in the Model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tr>
<td>$2\delta$</td>
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<tr>
<td>$v_1$</td>
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<tr>
<td>$v_2$</td>
<td>$0.46 \times 10^5$ m/s</td>
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<td>$m^f_e$</td>
<td>0.16 $m_e$</td>
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</tr>
<tr>
<td>$\alpha$</td>
<td>0.03 e nm</td>
</tr>
<tr>
<td>$k_0$</td>
<td>1.485 nm$^{-1}$</td>
</tr>
<tr>
<td>$d$</td>
<td>$40k_0^{-1} = 26.94$ nm</td>
</tr>
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</table>

![Fig. 1. Bulk energy dispersion in 1T'-MoS$_2$ two-dimensional material, $E_z=0$, for $k_x=0$ (solid line), $k_x=0.1k_0$ (dashed line), and $k_x=0.2k_0$ (dot-dashed line).](image1)

![Fig. 2. Bulk energy dispersion in 1T'-MoS$_2$ two-dimensional material, $k_x=0$, for $E_z=0$ (solid line), $aE_e\gamma\nu_e$ (dashed line) and $aE_e\gamma\nu_e$ (dot-dashed line).](image2)

![Fig. 3. Real (stars) and imaginary (line) parts of det($M$) computed at $k_x=0$, $E_z=0$, $d=40k_0^{-1}$. The bulk gap is seen at $E \approx \pm 0.005$, where the real part touches the OX axis from below. The subband energies are obtained from det($M$)=0. Topological edge states are seen in the bulk gap ($E \approx \pm 0.005$).](image3)
in the crossings of the curve with the axis OX. The bulk gap due to the spin-orbit interaction occurs at $E \approx \pm 0.065$. The value of the determinant approaches zero from negative values and touches it at a single point, when the energy $E$ touches the minimum (maximum) of the dispersion curve. Therefore, $k_1 = k_2$ and $k_3 = k_4$ and the determinant (5) is zero.

All other intersections with the OX axis correspond to subband energies. We clearly observe two roots in the gap at $E \approx \pm 0.005$. A close inspection shows that the wave vectors $k_j$ corresponding to these solutions are complex numbers. The wave functions corresponding to these solutions in the gap are located at an edge of the nanoribbon as shown in Fig.4 and Fig.5 for $k_y = 0.1 k_0$ and $E \approx \pm 0.005$, respectively. In contrast to [6], where only an exponential decay was predicted, the wave functions display both oscillations and decay. Although the structure of the Hamiltonians considered here and in [6] are similar, the actual parameters differ. In particular, here the spin-orbit gaps are open at the finite values of $k_y = \pm k_0$. This displacement of the bulk band’s minima from the Gamma-point at $k_y = 0$ is reflected in the oscillations of subband wave functions superimposed on the exponential decay.

The roots of the determinant for $|E| > 0.065$ correspond to the subbands with all $k_j$ real. The wave functions are delocalised through the width of the nanoribbon. Due to the strong non-parabolicity of the bulk dispersion, the positions of the subband minima and the subband dispersions can only be found by solving (5) numerically.

Fig. 6 shows the behavior of the determinant at $\alpha E_z = 0.7 v_2$. The gap at $E = \pm 0.02$ is reduced but not completely closed. However, due to the finite width of the nanoribbon, the edge modes seen at $E \approx \pm 0.02$ are already delocalized as the imaginary parts of two $k_j$ responsible for the localization at the edges is becoming zero. At the same time, the two solutions at $E \approx \pm 0.075$ split off from the traditional subbands set as two of their $k_j$ acquire an imaginary part. This happens due to the fact that, while the gap at $k_y = k_0$ shrinks with increasing $E_z$, the gap at $k_y = -k_0$ displays an opposite trend and becomes wider. Therefore, the lowest traditional subband initially outside of the gap enters the gap at $k_y = -k_0$ thus forcing the two roots to become complex.

The behaviour of the determinant at even higher electric field $\alpha E_z = 1.4 v_2$ is shown in Fig.7. As the field is larger than the
critical value field $E_z=\sqrt{2}\hbar k_0/\alpha$ at which there is no gap at $k_y=k_0$, the gap seen att $|E|<0.03$ is a direct gap. Therefore, as confirmed by the absence of zeroes of the determinant, no edge states are allowed in the gap. At the same time, there are already four subbands lying outside the direct gap at $k_y=k_0$ but still within the gap at $k_y\sim k_0$. While the solutions at $E\approx\pm0.09$ split off from the traditional subbands set in complete analogy to the situation in Fig. 6, the subbands at $E\approx\pm0.05$ originate in the edge states, which were continuously pushed outside of the gap at $k_y\sim k_0$.

Fig. 8 shows the dependence of the electron (hole) subband minima (maxima) $E^{(b)}_n$ on the electric field $E_z$. First, we note that the “bulk” gap in the nanoribbon defined as the difference between the extrema of the first traditional subbands (Fig.8, squares) shows signs of reduction, when the field is increased till $E_z=0.7v^2\hbar k_0/\alpha$, after which the trend is inverted. This behavior is in sharp contrast to that in wide ribbons in which the bulk gap closes and keeps increasing with increasing $E_z$. In contrast to the bulk case, the gap never closes and keeps increasing with $E_z$.

Second, with increasing $E_z$ the gap between the lowest electron and the highest hole-like subbands grows (Fig. 8, circles). As indicated in Fig.5 and Fig.6, all four $k_y$ contain an imaginary part for $E_z<0.7v^2\hbar k_0/\alpha$. This value is lower than the value $E_z<\sqrt{2}\hbar k_0/\alpha$ corresponding to the bands’ inversion in the bulk. The increasing gap between the edge-like subbands is reflected in the decrease of the corresponding nanoribbon ballistic conductance shown in Fig.9 (circles). Although the edge-like subbands give the leading contribution in the conductance $G$ (Fig.9, diamonds) computed as

$$G = \frac{2e^2}{h} \sum_{n} \left[ \frac{1}{\exp\left(\frac{\sqrt{2}E_n - E_F}{T}\right) + 1} - \frac{1}{\exp\left(\frac{\sqrt{2}E_n + E_F}{T}\right) + 1} \right],$$  

where $T$ is the temperature and $E_F$ is the Fermi energy, the role of the other subbands shown in Fig.9 by squares is non-negligible. The first two electron (hole) bulk-like subbands give similar contributions to the ballistic conductance totaling to 30%. However, all contributions to the total conductance $G$ rapidly decrease as a function of $E_z$ (Fig.9). This makes 1T'-MoS$_2$ potentially suitable for switching applications.

**ACKNOWLEDGMENT**

Financial support by the Austrian Federal Ministry for Digital and Economic Affairs and the National Foundation for Research, Technology and Development is gratefully acknowledged. A.-M.B.E.-S. was supported in part by project No. IN 23/2018 ‘Atom-to-Circuit modeling technique for exploration of Topological Insulator based ultra-low power electronics’ by the Centre for International Cooperation & Mobility (ICM) of the Austrian Agency for International Cooperation in Education and Research (OeAD).

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