Subbands in a nanoribbon of topologically insulating MoS$_2$ in the 1T$'$ phase

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A B S T R A C T

Continuous miniaturization has brought the feature size of silicon technology down into the nanometer scale, where performance enhancement cannot easily be achieved by further size reduction. The use of new materials 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 which are insensitive to scattering and thus suitable for energy efficient high-speed devices. Here, we evaluate the subband structure in a narrow nanoribbon of 1T$'$ molybdenum disulfide by employing an effective $k\cdot p$ Hamiltonian. Highly conductive topologically protected edge modes whose energies lie within the bulk band gap are investigated on equal footing with traditional electron and hole subbands. Due to the interaction between the edge modes at opposite sides, a small gap in their linear spectrum opens up 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 with negligible edge modes interaction. The gap between the traditional electron and hole subbands also increases with the perpendicular electric field. The increase of both gaps leads to a rapid decrease of the ballistic nanoribbon conductance and current with the electric field, which can be used for designing molybdenum disulfide nanoribbon-based current switches.

1. Introduction

Topological insulators (TIs) belong to a new class of materials characterized by highly conductive edge states which lie in the forbidden band gap of the bulk insulating material. In order to have such states in the gap, the bulk host material must possess an inverted band structure with the valence band edge above the conduction band edge. The existence of states with a gapless linear Dirac-like energy dispersion localized at the edge of a TI could be visualized as a result of restoring the standard band order with the conduction band above the valence band at the interface of the host bulk TI with a normal dielectric (air). The edge states are topologically protected by time-reversal symmetry, which results in electron propagation without backscattering. However, possessing robust conductive channels is only one requirement. To make a good switch it is necessary to efficiently control the current by suppressing it in the off-state as well as to abruptly change between the on- and off-states. A plausible option to control the current efficiently in a 2D TI is to modulate scattering by moving the Fermi level into and out of the bulk bandgap [2]. If the Fermi level lies in the gap, the electrons propagate through the topologically protected edge without backscattering (on-state). In contrast, the electrons from the edge states can scatter and backscatter strongly through the bulk states, if the Fermi level moves out the bandgap and lies in the bulk conduction band or in the valence band. Scattering suppresses the edge states’ current by more than two-orders of magnitude compared to the on-state current, thus paving the way to build an imperfect two-dimensional topological insulator field-effect transistor [2].

Recently it was found that the 1T$'$ phase of MoS$_2$, a well-known 2D material with high promise for future microelectronic devices [3], is a TI [4]. The inverted band structure predicted by \textit{ab-initio} calculations is well approximated by parabolas, with the conduction and valence bands having masses of $m_{\text{c}}(k)$ and their extrema separated by an inverted gap $2\delta$
In this article, we evaluate the subband structure in a narrow nanoribbon of 1T'-MoS2 TI as a function of the orthogonal electric field by employing an effective k-p Hamiltonian [4]. The gap between the non-topological bulk-like subbands never closes, instead increasing with the strength of the electric field. We find that a small gap in the spectrum of edge states opens at $k_x = 0$ and we show that it increases with an applied orthogonal electric field. The gap in the edge states is due to an interaction between the states located at opposite edges of a narrow nanoribbon [6]. As the gap increases with the electric field in a nanoribbon, it leads to a rapid decrease in the edge states’ ballistic conductance with increasing electric field, which is potentially suitable for switching. However, this is in contrast with recent findings [7]. We elucidate on the reason of the discrepancy and compute the ballistic conductance due to the edge-like modes for several nanoribbon widths.

2. Method

2.1. Effective Hamiltonian

The inverted band structure of 2D MoS$_2$ in a 1T' phase is well described by the parabolic dispersion relations

$$E_x(k_x, k_y) = -\delta - \frac{\hbar^2 k_x^2}{2m_x^*} - \frac{\hbar^2 k_y^2}{2m_y^*},$$  \hspace{1cm} (1)

and

$$E_z(k_x, k_y) = -\delta - \frac{\hbar^2 k_x^2}{2m_x^*} + \frac{\hbar^2 k_y^2}{2m_y^*} + \frac{\hbar^2 k_z^2}{2m_z^*} - \frac{E_z}{2},$$ \hspace{1cm} (2)

where $k = (k_x, k_y)$ is the wave vector, $E_x(k_x, k_y)$ and $E_z(k_x, k_y)$ refer to the valence and conduction bands, respectively, and $m_x^*, m_y^*$, and $m_z^*$ denote the effective masses [4]. The bands intersect at $k_y = \pm k_o$, where

$$k_o = \sqrt{\frac{4\delta}{\hbar^2 m_y^* m_x^*}}.$$ \hspace{1cm} (3)

Therefore, without taking spin–orbit interaction into account, the material is a semi-metal provided that the Fermi level crosses the intersection points. The spin–orbit interaction makes the conduction and the valence bands interact with each other, which opens gaps around the intersection points at $k_y = \pm k_o$. The effective Hamiltonian $H$ is written as [4,5]

$$H = \begin{pmatrix}
0 & 0 & -\alpha E_z - iv_x k_x & v_y k_y \\
0 & E_z(k_x, k_y) & v_x k_x & 0 \\
v_x k_x - \alpha E_z & v_y k_y & 0 & -\alpha E_z - iv_x k_x \\
v_y k_y & iv_x k_x - \alpha E_z & 0 & E_x(k_x, k_y)
\end{pmatrix},$$ \hspace{1cm} (4)

where $v_{x(2)}$ are the velocities defining the strength of the spin–orbit interaction and $\alpha$ describes the additional Rashba splitting between the bands due to the perpendicular electric field $E_z$ [5]. $E_z$ can manipulate and change the nature of the gap close to the degeneracy points at $k_y = \pm k_o$. The parameters [4] are listed in Table 1.

It is convenient to perform a canonical transformation of the Hamiltonian (4)

$$H(k) = A^{-1} H A$$ \hspace{1cm} (5)

by means of a unitary matrix $A$.

$$A = \frac{1}{2} \begin{pmatrix}
1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 \\
1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1
\end{pmatrix}.$$ \hspace{1cm} (6)

After the unitary transformation, the Hamiltonian $H'$ is in the block-diagonal form

$$H' = \begin{pmatrix}
0 & 0 \\
0 & H(-k)
\end{pmatrix},$$ \hspace{1cm} (7)

where $(Z^\dagger)$ stands for a conjugate transpose matrix $Z$. The possibility to express the Hamiltonian in the form (7) is a consequence of the time-reversal symmetry. To simplify the $2 \times 2$ Hamiltonian $H(k)$, we perform the additional transformation

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta$</td>
<td>0.33 eV</td>
</tr>
<tr>
<td>$v_x$</td>
<td>$3.87 \times 10^3$ m/s</td>
</tr>
<tr>
<td>$v_x$</td>
<td>0.46 $10^7$ m/s</td>
</tr>
<tr>
<td>$m_x^*$</td>
<td>0.5$m_e$</td>
</tr>
<tr>
<td>$m_y^*$</td>
<td>0.16$m_e$</td>
</tr>
<tr>
<td>$m_z^*$</td>
<td>2.48$m_e$</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>0.37$m_e$</td>
</tr>
<tr>
<td>$\delta$</td>
<td>0.33 eV</td>
</tr>
<tr>
<td>$k_o$</td>
<td>1.386 nm $^{-1}$</td>
</tr>
<tr>
<td>$d$</td>
<td>40$k_o^{-1} - 28.86$ nm</td>
</tr>
</tbody>
</table>
\[ \mathbf{H}(k) = B^{-1} \mathbf{H} B, \]  
with

\[
B = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 1 & 0 & 0 \\
1 & -1 & 0 & 0 \\
0 & 0 & 1 & 1 \\
0 & 0 & -1 & 1
\end{pmatrix}
\]  
(9)

The transformation (8), (9) preserves the block-diagonal structure (7). The upper 2 \times 2 block \( \mathbf{H}(k) \) is of the form

\[
\mathbf{H}(k) = \begin{pmatrix}
\delta + \frac{\hbar^2 k_x^2}{2 m_i^2} - \frac{\hbar^2 k_z^2}{2 m_i^2} & v_y k_z - a E_z + iv_z k_x \\
v_y k_z - a E_z - iv_z k_x & -\delta + \frac{\hbar^2 k_x^2}{2 m_i^2} + \frac{\hbar^2 k_z^2}{2 m_i^2}
\end{pmatrix}
\]  
(10)

If we measure energies in units of \( E_0 = 2\delta \) and the wave vectors \( k = (k_x, k_y) \) in units of \( k_0 \), the Hamiltonian (10) can be conveniently written in the dimensionless form

\[
\mathbf{H}(k) = \begin{pmatrix}
\frac{1}{2} - \frac{k_x^2 m_i^2}{m^2} - \frac{k_y^2 m_i^2}{m^2} & v_y k_z - a E_z + iv_z k_x \\
v_y k_z - a E_z - iv_z k_x & \frac{1}{2} + \frac{k_x^2 m_i^2}{m^2} + \frac{k_y^2 m_i^2}{m^2}
\end{pmatrix}
\]  
(11)

where \( m = \frac{m_0 m_i^2}{m^2} \) and \( v(2) \) are the dimensionless velocities. The Hamiltonian (11) possesses a similar form to the famous Hamiltonian \[8\] describing the quantum spin Hall effect in Hg/CdTe heterojunctions. However, the relation between the parameters is different, which results in the inverted band structure with the gap open by the spin-orbit interaction at a finite value of \( k_y = \pm k_0 \). The energy dispersion obtained from (11) and offset by

\[
\Delta E = \frac{1}{2} \frac{m_i^2 - m_0^2}{m^2}
\]  
(12)

is shown in Fig. 1 for \( k_z = 0 \). If the off-diagonal terms in (11) are zero, the dispersion curves intersect at \( k_y = \pm k_0 \) and \( E_z = 0 \). The spin-orbit interaction described by the off-diagonal terms opens a gap at the intersection of the valence and the conduction bands at \( k_y = \pm k_0 \), (Fig. 1, solid line).

When an electric field \( E_z \) along the OZ axis is applied, the gap at one of the minima reduces, completely closes (Fig. 1, dotted line), and opens again (Fig. 1, dot-dashed line) at large electric fields. The gap at large electric fields becomes direct and the bands are correctly ordered, so no edge states are possible within the bulk gap.

The gap also depends on \( k_x \) as shown in Fig. 2. The term which depends linearly on \( k_x \) enters in the off-diagonal terms in (11) similar to the term \( v_y k_z - a E_z \) \( \sigma_x \) linear in \( k_y \), where \( \sigma_x \) is the x-Pauli matrix. However, in contrast to the \( k_y \) term, the \( k_x \) term \(-iv_z k_x \sigma_y\) enters with \( \sigma_x \) Pauli matrix. As both orthogonal off-diagonal terms define the spin-orbit contribution to the gap \( \Delta \), it can be expressed as

\[
\Delta = (v_y k_z + (v_z k_x - a E_z) \sigma_y)^2.
\]  
(13)

Expression (13) explains the dependence of the gap on \( k_x \) seen in Fig. 2. It also explains, why the gap never closes, if the momentum \( k_y \) is nonzero.

2.2. Subband calculations

We consider a nanoribbon of width \( d \) confined along the OY axis. As the Hamiltonian (7) is block-diagonal, the eigenvalue problem of each block can be solved separately. Since the lower 2 \times 2 block \( \mathbf{H}(k) \) of the Hamiltonian (7) is the time-reversal of the upper block \( \mathbf{H}(k) \), the corresponding spin-down eigenwave function \( \psi(y) \) can be found from the spin-up solution for the upper block in (7) by the time-reversal symmetry transformation \( \psi(y) = -i \sigma_y \psi^*(y) \) [6], where \( \sigma_y \) is the Pauli matrix.

We therefore only focus on the solutions \( \psi(y) \) of the upper 2 \times 2 block Hamiltonian \( \mathbf{H}(k) \).

In the transverse direction only quantized values of the momentum \( k_y = k_y \) are allowed [9,10]. In addition, it is expected that at \( E_z = 0 \) two topologically protected edge states localize at opposite edges of the nanoribbon at an energy \( E \) within the gap which is opened at \( k_y = \pm k_0 \) by the spin-orbit interaction.

The subband wave functions \( \psi_{k_y}(y) \) in the quantization direction have the general form [9]

\[
\psi_{k_y}(y) = \sum_{j=1}^{4} A_j \begin{pmatrix} a \\ b \end{pmatrix} \exp(i k_j y),
\]  
(14)

where \( A_j \) are some expansion coefficients, the wave numbers \( k_1, \ldots, k_4 \) are the roots of \( \epsilon(k_x, k_y) = E \), where \( \epsilon(k_x, k_y) \) is the bulk dispersion, and the spinor \( (a, b)^T \) is an eigenvector of (11) with

\[
a = v_y k_x - a E_z + iv_z k_x,
\]  
(15a)

\[
b = -\frac{1}{2} \left( \frac{k_x^2 m_i^2}{m^2} + \frac{k_y^2 m_i^2}{m^2} \right) + E.
\]  
(15b)
Setting the wave function at both edges to zero yields the quantization condition
\[ \det(M) = 0, \] (16)
where the matrix \( M = (m_1 \ m_2 \ m_3 \ m_4) \) is composed of the column vectors \( m_i \) defined as
\[ m_i = \begin{pmatrix} a \\ b \\ \exp(i k d) \\ \exp(i k d) \end{pmatrix} \] (17)
From the condition \( \det(EI - H) = 0 \) a quartic equation for \( k_x \) is obtained:
\[ k_x^4 + c k_x^2 + c k_x + c_0 = 0. \] (18)
A simultaneous solution of (16) and (18) is found numerically using the Newton method. We define the unknown vector as \( x = (k_1, k_2, k_3, k_4, E)^T \) and treat \( k_x \) as an input parameter. By means of Vieta’s formulas a nonlinear equation system of the form \( F(x) = 0 \) can be set up, where the vector-valued function \( F \) is composed of the following components:
\[ F_1 = k_1 k_2 k_3 k_4 - c_0 \]
\[ F_2 = k_1 k_2 k_3 + k_1 k_2 k_4 + k_1 k_3 k_4 + k_2 k_3 k_4 + c_1 \]
\[ F_3 = k_1 k_2 + k_1 k_3 + k_2 k_3 + k_1 k_4 + k_2 k_4 + k_3 k_4 - c_2 \]
\[ F_4 = k_1 + k_2 + k_3 + k_4 \]
\[ F_5 = \det(M). \] (19)
In a typical band structure calculation, one chooses an initial point \( (k_0, E) \). To have the Newton iteration converge to an energy close to its initial value and to prevent jumps to some remote subbands, the update vector has to be damped. During the Newton iteration, \( E \) is allowed to assume real values only, whereas the \( k_x \) are complex.

Fig. 3 displays the behavior of the real part (the imaginary part is zero for \( E_0 = 0 \)) of the determinant as a function of energy, for \( k_x = 0 \). We are interested in the crossings of the curve with the line \( E = 0 \). The bulk gap due to the spin–orbit interaction occurs at \( E \approx \pm 0.06 \). The value of the determinant approaches zero from negative values and touches it at a single point. If we now draw a horizontal line at an energy \( E \) in Fig. 1 and start moving \( E \) from negative values up to positive values, it enters into the gap at \( E \approx -0.06 \) and leaves the gap at \( E \approx 0.06 \) for \( E_0 = 0 \) (Fig. 1, solid lines). Therefore, at these energies, the constant energy \( E \) horizontal line touches the maximum (minimum) of the dispersion curves. At these points \( k_1 = k_2 \) and \( k_3 = k_4 \), which ensures the determinant (16) is zero.

Although (16) is zero at these energies, the roots discussed above must be excluded from the consideration of subbands in a nanoribbon. Indeed, (16) is zero because at least two of the columns (17) are identical due to \( k_1 = k_2 \) and/or \( k_3 = k_4 \). In this case the wave function (14) contains only three coefficients \( A_j \) which are determined by zero boundary conditions. As the wave function (14) contains two components, and each of the components must be zero at the edges of the nanoribbon, we have an overdetermined system of four linear equations for these three coefficients \( A_j \). The only solution in this case is the trivial one, where the wave function is zero everywhere. Therefore, these roots do not correspond to subbands and must be disregarded. We note here that these solutions were wrongly assigned in [7] to subbands, which resulted in an incorrect interpretation of the results as we discuss later in detail.

All other intersections with the line \( \det(M) = 0 \) correspond to subband energies. We clearly observe two roots located in the gap at \( E \approx \pm 0.005 \). A close inspection shows that the wave numbers \( k_x \) corresponding to these two solutions are complex. The wave functions for the spin-up case corresponding to these solutions in the gap are located at an edge of the nanoribbon as shown in Figs. 4 and 5 for \( k_x = 0.1 k_0 \) and \( E \approx \pm 0.005 \), respectively. The electron (\( E \approx 0.005 \)) wave function shown in Fig. 4 is localized at the left edge of the nanoribbon. Due to time-reversal symmetry, the electron wave function square for the opposite spin orientation (spin down) and for \( k_x = -0.1 k_0 \) coincides with the one shown in Fig. 4. The spin-up wave function is localized at the right edge of the nanoribbon at \( k_x = -0.1 k_0 \). It is a mirror symmetric to the wave function shown in Fig. 4 relative to the center of the nanoribbon.

The wave function for holes (\( E \approx -0.005 \)) in the spin-up case is shown in Figs. 5. It is located at the opposite edge of the wave function for electrons. Following similar arguments, the hole wave functions for the spin-down case and \( k_x = \pm 0.1 k_0 \) can be easily obtained. The wave function for the spin-down case and \( k_x = -0.1 k_0 \) is localized at the left edge, while the wave function for the spin-up case and \( k_x = -0.1 k_0 \) coincides with the one shown in Fig. 5. We note that only the part of the wave function describing the subbands are similar, while the complete wave function includes the plane wave factor describing the propagations in opposite directions along the OXaxis.

In contrast to [6], where only an exponential decay of the edge states was predicted, the wave functions shown in Figs. 4 and 5 display both oscillations and decay. We also note that the period of the electron wave function oscillations is not equal to that of the hole function and is a bit
shorter. This is because the minima of the hole bands in Fig. 1 are at slightly smaller wave vectors than those of the electron bands. This displacement of the bulk band’s minimum from the Gamma-point at \( k_y = 0 \) is reflected in the oscillations of subband wave functions superimposed on the exponential decay. This displacement is due to different parameters in the otherwise similar Hamiltonian considered in [6], where no oscillations were predicted.

The roots of the determinant for \( |E| > 0.06 \) correspond to subbands whose \( k_j \) are all real. The wave functions are delocalized throughout the width of the nanoribbon. Due to the strong non-parabolicity of the bulk dispersion, the positions of the subband minima and their dispersions can only be found by solving (16) and (18) numerically.

Fig. 6 shows the behavior of the determinant at \( aE_e = 0.7\nu_2 k_0 \). In this case the gap at \( \nu = 0 \) determined by the extrema of the bulk band structure and the zeroes of (16) at \( E \approx \pm 0.02 \) is reduced, but not completely closed. The extrema of the bulk band structure at \( k = -k_0 \) are clearly seen as zeroes of (16) at \( E \approx \pm 0.1 \).

The edge modes appear close to \( E \approx \pm 0.02 \). At this particular value of the electric field the edge modes are about to leave the gap and become delocalized as the imaginary parts of two out of four \( k_j \) responsible for the localization at the edges become zero. The two solutions at \( E \approx \pm 0.075 \) have split off from the traditional bulk-like subbands. Their wave functions’ behavior is qualitatively different from the bulk subbands behavior as two out of four of their \( k_j \) acquire an imaginary part. This happens because the gap at \( k_x = k_0 \) shrinks with increasing \( E_x \), the gap at \( k_y = -k_0 \) exhibits an opposite trend and becomes wider. Therefore, the lowest traditional subband, whose energy is initially outside of the gap, enters the gap at \( k_y = -k_0 \) thus forcing the two roots to become complex.

The behavior of the determinant at an even higher electric field \( aE_e = 1.4\nu_2 k_0 \) is shown in Fig. 7. As the field is larger than the critical field \( aE_e = \nu_2 k_0 \), at which there is no gap at \( k_y = k_0 \), the gap seen at \( |E| < 0.03 \) is now a direct gap. Therefore, no edge states can exist within the direct gap, which is confirmed by the absence of zeroes of the determinant within the direct gap \( |E| < 0.03 \). There are four subbands lying outside the direct gap at \( k_y = k_0 \) but still within the gap at \( k_y = -k_0 \) defined by zeroes of (16) due to the bulk band extrema at \( E \approx -0.14 \) and \( E \approx 0.15 \), respectively. While the solutions at \( E \approx \pm 0.09 \) are split off from the traditional subbands, in complete analogy to the situation in Fig. 6, the subbands at \( E \approx \pm 0.05 \) originate from the edge states which were continuously pushed outside of the gap at \( k_y = -k_0 \).

3. Subbands dispersions in nanoribbon

The dispersions of several electron and hole subbands are shown in Fig. 8. The width \( d \) of the nanoribbon along the \( OY \) axis equals \( d = 40k_0^{-1} \approx 28.86 \) nm. The lowest electron/topmost hole subbands possess a linear dispersion. This distinguishes the subbands from traditional subbands in silicon films. The energies of these subbands lie in the bulk band gap (Fig. 1, solid lines). The subbands correspond to the topologically protected edge modes as their wave functions are localized at the edges [11].

A close inspection reveals that a small gap has opened at \( k_x = 0 \) reflecting the fact that the topological states located at the two opposite edges of the nanoribbon start interacting at \( k_x = 0 \) [6]. At larger \( k_x \), the coupling between the edge states becomes insignificant, because the edge states located at opposite edges (Figs. 4 and 5) propagate in opposite directions and do not interact.

Fig. 9 shows the subbands’ dispersions at an electric field of \( E_x = \frac{\nu_1 k_0}{\nu_2} \). The gap between the bulk bands would be closed at this field value in an infinitely large system (Fig. 1). However, in contrast to the bulk dispersion, the splitting between the lowest electron and topmost hole subband in a narrow nanoribbon remains finite and actually increases compared to the case without electric field. The splitting becomes even larger at higher electric fields as demonstrated in Fig. 10. As the gap between the lowest electron/topmost hole subband grows with the electric field, their dispersions change from a linear to a quadratic behavior in a broader interval of \( k_x \).

To obtain the higher electron/hole subbands’ other roots outside of the bulk gap at \( E_x = 0 \) must be evaluated. We note that an approximation
of parabolic bands could only be applied to very high energy subbands, as close to the bulk gap the dispersion relation is highly nonparabolic, so (16) must be resolved numerically. Let us define the “bulk” gap in a nanoribbon of a finite width as the gap between the first traditional, non-topological electron and hole subband. Obviously, the gap does not close at $E_z = \nu_2 k_0^2 \alpha$ (Fig. 9) and keeps increasing for larger electric fields (Fig. 10).

Fig. 11 shows the dependence of the electron (hole) subband minima (maxima) $E_n^e$ ($E_n^h$) on the electric field $E_z$. In contrast to the bulk case (shown with dashed lines), the gap never closes and keeps increasing with $E_z$.

Fig. 10. Subbands in a nanoribbon of the width $d = 40/k_0$, $E_z = 0$. The subband with an almost linear dispersion (in red) corresponding to the topologically protected edge state is clearly seen. A small gap is opened at $k_y = 0$ due to the interaction between the edge modes at opposite edges of the nanoribbon. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 8. Subbands in a nanoribbon of the width $d = 40/k_0$, $E_z = 0$. The subband with an almost linear dispersion (in red) corresponding to the topologically protected edge state is clearly seen. A small gap is opened at $k_y = 0$ due to the interaction between the edge modes at opposite edges of the nanoribbon. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 9. Subband energies at $\alpha E_z = \nu_2 k_0^2$, when the gap at $k_y = k_0$ is closed, see Fig. 1, dotted lines. Red lines describe subbands with two real and two complex $k_j$, while blue subbands have four real $k_j$ real at small $k_y$. No subbands with linear dispersion are observed. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 11. Dependence of electron ($E > 0$) and hole ($E < 0$) subband minima (maxima) on the electric field $E_z$, when the direct gap is opened at $k_y = k_0$, see Fig. 1, dot-dashed lines. Now six subbands (in red) at small $k_y$ acquire two real and two complex $k_j$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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Dashed lines. We note that at the value $E_z \approx 0.7 \nu_2 k_0^2$ of the electric field two of the four values of the wave vectors defining the wave function of edge-localized solutions become real (Fig. 6), so the edge wave function (14) becomes “delocalized” across the width of the nanoribbon.

Let us now compare the dispersions shown in Figs. 9 and 3c from [7]. The striking distinction is the absence of the linear bulk-like dispersion which is attributed to the edge modes in [7]. Although the determinant (16) is zero along this linear dispersion, these solutions are not related to the edge modes. These zeroes of (16) appear at the extrema of the bulk dispersion. At the extrema with energy $E$, the two roots $k_j$ of the equation $\epsilon(k_x, k_j) = E$ are equal. It immediately causes the determinant (16) to become zero, because the two columns (17) are identical. In the case of $\alpha E_z = \nu_2 k_0^2$, the bulk dispersion is linear as seen in Fig. 1. Although these solutions give zeroes of (16), they have nothing to do with the subband solutions satisfying (16) because of the boundary conditions, the subband wave function...
must satisfy. Therefore, the linear bulk-like modes seen in Fig. 3c of [7] must be disregarded as they do not correspond to the subbands. The subband spectrum is gapped as shown in Fig. 9.

Our conclusion is based on the assumption that the wave function is in the form (14) valid when all four of the roots \( k_j \) of the equation \( \epsilon(k_x, k_y) = E \) are different. Although it is not the case at isolated points where the two roots \( k_j \) of the equation \( \epsilon(k_x, k_y) = E \) coincide, it does not affect the generality of our result. As we prove in the Appendix, the zero boundary conditions on the wave function can only be satisfied at a very specific, discrete set of nanoribbon widths. The set of widths is different for any \( k_x \) momentum. As we show in the Appendix, for a fixed nanoribbon width, the boundary conditions can only be satisfied at isolated \( k_y \) points. A continuous solution does not exist and, therefore, no subband with a continuous dispersion corresponding to the degenerate roots \( k_j \).

In order to further demonstrate the fact that the linear dispersion observed in Fig. 3c of [7] does not correspond to any subband, we plot the lowest electron/topmost hole subbands’ energy dependence on the electric field for several nanoribbon widths in Fig. 12. The gap between the lowest electron and topmost hole subband increases with the nanoribbons width decreased. The transition, when the confined edge-like states becomes delocalized along the whole width of the nanoribbon, is determined by the intersection of the corresponding dispersions with the dashed lines in Fig. 12 showing the dependence of the bulk bands on \( E_z \). As is seen from Fig. 12, this transition shifts towards lower electric field values for narrow nanoribbons.

At the same time, the minimum and maximum of the bulk bands at \( k_y = k_0 \), incorrectly attributed in [7] to the edge-like modes and shown in Fig. 12 with green dashed lines, display a linear dependence on the electric field but do not depend on the nanoribbon width. This confirms our claim that these linear solutions due to the extrema of the bulk dispersion must be disregarded for describing the quantized subbands in a nanoribbon.

4. Ballistic conductance

An increase in the energy separation between the electron and hole subbands (Fig. 11) in nanoribbons as a function of a perpendicular electric field is reflected in a rapid decrease of the nanoribbon ballistic conductance [12]. The ballistic conductance is computed as

\[
G = \frac{2e^2}{h} \sum_{j} \left[ \frac{1}{\exp \left( \frac{E_z - E_{Fj}}{k_B T} \right) + 1} + \frac{1}{\exp \left( \frac{E_{Fj} - E_z}{k_B T} \right) + 1} \right],
\]

where \( T \) is the temperature and \( E_F \) is the Fermi energy. If the Fermi energy is close to the middle of the gap (\( E_F \approx 0 \)), the edge-like subbands dominate the conductance \( G \) [12]. The role of the traditional subbands is non-negligible as the two lowest (topmost) electron (hole) bulk-like contribute 30% of the ballistic conductance. However, all contributions to the total conductance \( G \) rapidly decrease as a function of \( E_z \). This makes 1T-MoS2 promising for switching applications [12].

Let us evaluate the ballistic conductance due to the lowest electron and topmost hole edge-like subband only and compare it with the results of [7] for different nanoribbon widths. As it is seen in Fig. 13, the ballistic conductance decreases with the perpendicular electric field. This is in sharp contrast with [7] where, after an initial decrease, the ballistic conductance starts increasing at higher fields. The increase of the ballistic conductance in [7] is the consequence of the extrema of the bulk dispersion. Although (16) is satisfied, these roots are not due to the subbands and must be disregarded as demonstrated above. Therefore, the ballistic conductance due to the lowest electron/topmost hole subband decreases with increasing electric field \( E_z \).

5. Conclusion

The subband structure in a narrow nanoribbon of 1T molybdenum disulfide as a function of an out-of-plane electric field is evaluated by employing the effective four-band \( k \cdot p \) Hamiltonian. It is shown that by an appropriate unitary transformation the Hamiltonian can be recast in a convenient block-diagonal form used to describe topological insulators. In a confined geometry of a nanoribbon the Hamiltonian describes the complete subband structure including topologically protected edge modes. In contrast to the behavior in a wide nanoribbon, where the bulk gap closes at a certain field value and becomes direct at higher values of the electric field, the gap between the traditional lowest electron and highest hole subband never closes and increases with the perpendicular electric field. The increase in the separations between the electron and hole subbands leads to a substantial decrease of their contribution to the total ballistic conductance and current as a function of the perpendicular electric field.

![Fig. 12. Dependence of the lowest electron and topmost subbands on the perpendicular electric field in nanoribbons of different widths. The separation gap between the subbands increases with \( E_z \). The dependence of the bulk bands minimum and maximum at \( k_y = k_0 \) on \( E_z \) is shown with dashed lines.](image1)

![Fig. 13. Ballistic conductance due to the lowest electron-topmost hole subband in a 1T-MoS2 nanoribbon of different widths. The ballistic conductance keeps decreasing with \( E_z \) increased.](image2)
The edge modes’ energies lie in the bulk gap. Their dispersion relations are almost linear as a function of the momentum along the nanoribbon and their wave functions are localized at the edges and display damped oscillation. Due to the interaction of the edge modes located at the opposite sides of a narrow nanoribbon, a small gap in their linear dispersion spectrum opens at momenta close to zero. The gap increases rapidly with a perpendicular electric field resulting in a substantial decrease of the contribution due to the edge modes in the ballistic conductance. As the ballistic conductance decreases substantially, varying the electric field is shown to be an attractive option for designing molybdenum disulfide nanoribbon-based current switches.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix

In order to find the subbands in a nanoribbon of the widths \(d\) along the \(OY\) axis we must solve the Schrödinger equation with the Hamiltonian (11) for the wave function \(\psi_{ik}(y)\) and energy dispersion \(E(k_y)\).

\[
(H - E(k_y)I)\psi_{ik}(y) = 0
\]  
(A1)

The wave function must satisfy zero boundary conditions at both edges of the nanoribbon.

\[
\psi_{ik}(y = 0) = \psi_{ik}(y = d) = 0
\]  
(A2)

(A1) is a second-order differential equation. To find its general solution as a function of \(y\), we have to determine the \(k_y\) roots of the characteristic equation

\[
\det(H - E I) = 0
\]  
(A3)

It is equivalent to finding the \(k_y\) roots of the equation

\[
\epsilon(k_x, k_y) = E,
\]  
(A4)

where \(\epsilon(k_x, k_y)\) is the bulk energy dispersion of an infinite sheet and \(k_j, j = 1, \ldots, 4\) are the four \(k_y\) roots of the characteristic Eqs. (A3) and (A4).

If all four roots \(k_j\) are different, the wave function is of the form (14). However, when any two of the roots \(k_1 = k_2 = k\) are equal, the wave function is of the form

\[
\psi_{ik}(y) = (A_1 + A_2 y) \left( \begin{array}{c} a \\ b \end{array} \right) \exp(ik_y y) + \sum_{j \neq k} A_j \left( \begin{array}{c} a_j \\ b_j \end{array} \right) \exp(ik_j y),
\]  
(A5)

where the spinor \((a_j, b_j)^T\) is defined by (15) with \(k_j = k_y\).

In order to have a nontrivial solution satisfying (A2) the following determinant must be zero:

\[
\left| \begin{array}{cccc}
 a & 0 & a_3 & a_4 \\
 b & 0 & b_3 & b_4 \\
 a \exp(ikd) & ad \exp(ikd) & a \exp(ikd) & a \exp(ikd) \\
 b \exp(ikd) & bd \exp(ikd) & b \exp(ikd) & b \exp(ikd)
\end{array} \right| = 0
\]  
(A6)

By replacing the first column with a linear combination of the first and second column the determinant (A6) reduces to

\[
\left| \begin{array}{ccc}
 a & 0 & a_3 \\
 b & 0 & b_3 \\
 0 & a \exp(ikd) & a \exp(ikd) \\
 0 & b \exp(ikd) & b \exp(ikd)
\end{array} \right| = 0.
\]  
(A7)

From here we obtain:

\[
\frac{(ba_1 - ab_1) \exp(ikd)}{(ba_4 - ab_4) \exp(ikd)} = \frac{ba_4 - ab_4}{(ba_1 - ab_1) \exp(ikd)} = 0
\]  
(A8)

We introduce

\[
c_1 = ba_1 - ab_1,  
\]  
(A9a)

\[
c_2 = ba_4 - ab_4.
\]  
(A9b)

Because the spinors \((a, b)^T\) and \((a_j, b_j)^T, j = 3, 4\) evaluated at nonequal roots \(k_1 = k_2 = k\) and \(k_j, c_{1,2}\) in (A9) are always nonzero.
\[c_1 c_2 \exp(i k d) = c_1 c_2 \exp(i k d). \quad (A10)\]

It is satisfied only, if
\[\exp(i k d) = \exp(i k d). \quad (A11)\]

If \(k_i\) is different from \(k_0\), \((A11)\) is equivalent to
\[d_k = \frac{2 \pi n}{|k_3 - k_4|}, \quad n = 1, 2, \ldots. \quad (A12)\]

Because \(k_3, k_4\) are uniquely defined by the extremum of the energy \(E\) of the bulk dispersion \(\varepsilon(k, k) = E\) at fixed \(k_3\) and \(E_k\), \((A12)\) is an equation for \(d_k\). As \(d_k\) depends on \(k_4\), these discrete isolated solutions do not correspond to any subband in a ribbon of the fixed width \(d\) and must be disregarded.

If \(k_3 = k_4\) which may only happen at \(E_k = 0\), \(k_3 = -k\), and the wave function has the form
\[\psi_{k_3}(y) = (A_1 + A_2 y) \begin{pmatrix} a \\ b \end{pmatrix} \exp(i k y) + (A_1 + A_2 y) \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \exp(i k y). \quad (A13)\]

This results in the following determinant:
\[\begin{vmatrix} a & 0 & a_1 \\ b & b_1 & 0 \\ 0 & a & a_1 \\ 0 & b & b_1 \end{vmatrix} = -(ab_1 - a_1 b)^2 \quad (A14)\]

As the spinors \((a, b)^T\) and \((a_3, b_3)^T\) are the eigenfunctions of \((11)\) with different \(k_3 = -k\), \((A13)\) can have only accidental isolated roots, see e.g. \((15)\). Therefore, no subband exits with a continuous dispersion corresponding to the degenerate roots \(k_j\).

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