Corrigendum

Corrigendum: Numerical analysis of surface and edge states in slabs, stripes, rods and surface steps of topological insulators (2018 J. Phys.: Condens. Matter 30 485301)

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The second sentence of section 2
‘We use the following set of parameter values corresponding to Bi$_2$Se$_3$ energy structure: $M = 0.28$ eV, $C = -0.0068$ eV, $A_1 = 0.22$ eV Å, $A_2 = 0.41$ eV Å, $B_1 = 0.1$ eV Å$^2$, $B_2 = 0.566$ eV Å$^2$, $D_1 = 0.013$ eV Å$^2$, $D_2 = 0.196$ eV Å$^2$ [12].’

Should read
‘We use the following set of parameter values corresponding to Bi$_2$Se$_3$ energy structure: $M = 0.28$ eV, $C = -0.0068$ eV, $A_1 = 0.22$ eV nm, $A_2 = 0.41$ eV nm, $B_1 = 0.1$ eV nm$^2$, $B_2 = 0.566$ eV nm$^2$, $D_1 = 0.013$ eV nm$^2$, $D_2 = 0.196$ eV nm$^2$ [12].’

This misprint does not affect the rest of the paper. All the calculations have been done with correct numbers.

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Numerical analysis of surface and edge states in slabs, stripes, rods and surface steps of topological insulators

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Abstract

By numerically solving the effective continuous model of a topological insulator with parameters corresponding to the band structure of the topological insulator Bi$_2$Se$_3$, we analyze possible appearance of one-dimensional states in various geometries. Massless Dirac fermions are found at the edges of thin ribbons with surface oriented not only along the van der Waals gap but also in the perpendicular direction. Thick rods and slabs with surface steps host massive modes localized on surface faces. We argue that the origin of the massive modes is due to the difference in the Dirac point energy of adjacent faces. The absence of one-dimensional states near edges of a large rectangular rod and surface steps is demonstrated.

Keywords: topological insulator, edge states, surface step, bound state, Bi$_2$Se$_3$, nanoribbon

(Some figures may appear in colour only in the online journal)
2. Model and calculation methods

In the framework of the effective continuous model proposed by Zhang et al [12] the states of a TI near the Γ-point can be described by a Hamiltonian.

\[ H = E_0(k) + \begin{pmatrix} M(k) & A_1 k_x & 0 & A_2 k_z \\ A_1 k_x & -M(k) & 0 & 0 \\ 0 & A_2 k_z & M(k) & -A_1 k_x \\ A_2 k_z & 0 & -A_1 k_x & -M(k) \end{pmatrix}, \]  

where \( k_\pm = k_x \pm ik_z \), \( E_0(k) = C + D(k_x^2 + D_2(k_y^2 + k_z^2), \)

\( M(k) = M - B_1 k_x^2 - B_2(k_y^2 + k_z^2) \) and \( A_1, A_2, B_1, B_2, C, D_1, D_2 \) are numerical parameters. We use the following set of parameter values corresponding to Bi2Se3 energy structure: \( M = 0.28 eV, \quad C = -0.0068 eV, \quad A_1 = 0.22 eV, \quad A_2 = 0.41 eV, \quad B_1 = 0.1 eV, \quad B_2 = 0.566 eV, \quad C_1, D_1 = 0.013 eV, \quad D_2 = 0.196 eV, \quad 12]. z \) is the direction transverse to the cleavage surface of Bi2Se3 and the x-y plane is parallel to it.

We will study here the energy structure of slabs, rods and ribbons, and steps with various orientations. In the case of rods, ribbons and steps running along the y axis we are considering systems translationally invariant along the x axis, so \( k_y \) is conserved and two remaining wave vector components are replaced by their operators \( k_x \rightarrow -i\partial_x \) and \( k_z \rightarrow -i\partial_z \). For each \( k \) we treat the corresponding resulting Dirac equation as a two-dimensional equation for a continuous wave function \( \psi^{(\alpha)}(x, z) \), where \( \alpha = 1, ..., 4 \) is the index of the wave function component, and solve it by a standard finite difference method. Specifically, we introduce a rectangular grid \( x_n = n \lambda h, \quad z_m = m \lambda h, \) with \( n = 0, ..., N - 1, \quad m = 0, ..., M - 1 \), typically \( h = 0.4 - 0.5 \) nm, \( \lambda = 0.2 - 0.4 \) nm and \( N \times M = 1000 - 3000 \). Note that this grid is not connected with the actual crystalline lattice of the material under consideration. Then we discretize the wave function \( \Psi_{n,m}^{(\alpha)} = \psi^{(\alpha)}(x_n, z_m) \). The differential operators are replaced by central finite differences

\[ \partial_x \psi^{(\alpha)}(x_n, z_m) \rightarrow (\psi^{(\alpha)}(x_{n+1}, z_m) - \psi^{(\alpha)}(x_{n-1}, z_m))/2h_x, \]

\[ \partial_y \psi^{(\alpha)}(x_n, z_m) \rightarrow (\psi^{(\alpha)}(x_n, z_{m+1}) - \psi^{(\alpha)}(x_n, z_{m-1}))/2h_z, \]

\[ \partial_z \psi^{(\alpha)}(x_n, z_m) \rightarrow (\psi^{(\alpha)}(x_{n+1}, z_m) - 2\psi^{(\alpha)}(x_n, z_m) + \psi^{(\alpha)}(x_{n-1}, z_m))/h_x^2, \]

\[ \partial_z \psi^{(\alpha)}(x_n, z_m) \rightarrow (\psi^{(\alpha)}(x_n, z_{m+1}) - 2\psi^{(\alpha)}(x_n, z_m) + \psi^{(\alpha)}(x_n, z_{m-1}))/h_z^2. \]

We model the surface with zero boundary conditions. For the rods and ribbons that means putting \( \psi^{(\alpha)}_{-1,m} = \psi^{(\alpha)}_{N+1,m} = \psi^{(\alpha)}_{n,m} = 0 \) in the above expressions. For the surface steps of height \( L_s = Sh \) the boundary conditions look as follows

\[ \psi^{(\alpha)}_{-1,m} = 0, \quad m = 0, ..., S - 1 \]

\[ \psi^{(\alpha)}_{L_s, m} = 0, \quad m = S, ..., M - 1 \]

\[ \psi^{(\alpha)}_{N,m} = 0, \quad m = 0, ..., M - S - 1 \]

\[ \psi^{(\alpha)}_{n,m} = 0, \quad m = 0, ..., M - S - 1 \]

\[ \psi^{(\alpha)}_{n,-1} = 0, \quad n \neq 0, M. \]
This reduces the problem to a system of linear algebraic equations for $4NM$ variables $\Psi_{n,m}^{(\alpha)}$. The LDOS is defined as $\rho(r,E) = \sum_i |\psi_i(r)|^2 \delta(E - E_i)$, where $\psi_i(r)$ and $E_i$ are the wave function and the energy of the $i$th state. Partial LDOS is obtained by summation not over all values of $i$ but a subset thereof. The treatment of rods, ribbons and steps running along the $z$ axis is analogous. In the case of an infinite slab two momentum projections are good quantum numbers and we solve only a 1D equation numerically.

3. Results

3.1. Infinite slab

Analysis of the properties of a slab allows us to verify the method and the approximation used.

Figure 1 shows the dispersion curves for the surface and bulk states obtained by solving equation (1) for different surface orientations for a 25 nm thick slab. Such a thickness is sufficient to reduce the effect of surface state hybridization to a negligible level. We have here three different energy regions: valence band states region $E \lesssim -0.19$ eV, surface states region $-0.19 \lesssim E \lesssim 0.28$ eV, and the conduction band region $E \gtrsim 0.28$ eV. The Fermi velocity for $x$–$y$ plane $v_F = A_2 \sqrt{1 - (D_1/B_1)^2} \approx 0.4$ eV nm$^{-1}$ [33] is close to the value observed experimentally [48] whereas the bulk energy gap is slightly above the experimental one (0.3 eV [48, 49]). Another difference is the position of the Dirac point inside the bulk energy gap: it is located approximately in the middle of the energy gap for the $x$–$y$ face, whereas both ARPES and STS measurements give approximately 0.1 eV above the valence band. Anisotropy of the energy structure manifests itself in the elliptic shape of the constant-energy surfaces (figure 1(b)). The model also reproduces different Dirac point positions on different faces, in agreement with $ab$ initio calculations [36].

Decrease in the slab thickness leads to hybridization of the surface states. As a result, an energy gap is opened for the surface states. The bulk energy gap also increases due to the quantum size effect. Figure 2 shows the gap value as a function of the slab thicknesses (blue and red curves) and ribbon width for critical thickness ribbons.

![Figure 1. Dispersion laws for a 25 nm thick slabs with non-overlapping surface states. (a) Surface orientation along the $x$–$y$ plane; (b) along $y$–$z$ plane.](image1)

![Figure 2. Energy gap as a function of the slab thicknesses (blue and red curves) and ribbon width for critical thickness ribbons.](image2)
imaginary parts in the exponents $\lambda_1$ and $\lambda_2$ defining the decay of the surface states wave functions $\Psi(z) \propto e^{\lambda_1/z} + e^{\lambda_2/z}$ in the effective continuous model [33]. Such oscillations correspond to periodical band inversion [32] and are responsible for the development of a 2D topological insulator phase in certain critical regions of slab thickness (see below).

3.2. Rectangular rod

Analysis of the states of a rectangular rod allows us to clarify the question of possible appearance of edge states in thin layers of topological insulators, as well as in the corners of a thick and wide one. Let us consider a rod directed along the $y$ axis. $k_x$ is now not a good quantum number any more, but $k_y$ is. Figure 4(a) shows the dispersion curves for electron states in a $10 \times 30$ nm$^2$ rod. Here both the rod’s thickness and width are big enough to exclude overlapping of the surface states of opposite faces. So the bulk energy gap is approximately the same as in the case of a thick slab, but the surface states are quantized and a small energy gap develops. The quantization is determined by the effective perimeter of the rod cross-section and obeys the following equations

$$\begin{cases} L_x k_x + L_z k_z = \pi \left( N + \frac{1}{2} \right) \\ k_y v_F + E_{D_{xy}} = k_z v_F + E_{D_{yz}}, \end{cases}$$

(accounting for face- and direction-dependent $v_F$, Berry phase and dependence of the Dirac point position on face orientation. For the sake of simplicity we neglect here the weak energy dependence of $v_F$. The difference between the energy quantization levels of the surface states with small wavevectors is then

$$\Delta E = \frac{\pi v_F v_F}{v_F L_x + v_F L_z}. \quad (3)$$

Alternatively, it can be rewritten as

$$\Delta E = \frac{2\pi v_F v_F}{P_{\text{eff}}}, \quad (4)$$

where $P_{\text{eff}} = 2L_x + \frac{2\pi}{v_F} L_z$ is the effective perimeter of a rod. This is an approximate formula not taking into account the depth distribution of the surface states.

Figure 3 maps the value of the energy gap in the $\Gamma$ point versus $L_x$ and $L_z$. The map consists of a relatively flat plateau at $(L_x \gtrsim 15 \text{ nm}, L_z \gtrsim 5 \text{ nm})$ and two deep gorges along the $x$ and $z$ axes resulted from the oscillating character of the energy gap. The plateau has a slope shown by the level lines. They correspond to constant values of the effective perimeter, $L_x + 1.8 L_z = \text{const}$, in agreement with equation (4). Calculations for the rod running in the $z$ direction give analogous results.

As noted above, the Dirac point position depends on face orientation. In the model discussed here this splitting is $\approx 0.06 \text{ eV}$ (figure 4). As a result, the motion of the Dirac electrons from face to face occurs through a set of rectangular potential wells. Therefore, electron states can be bound to certain faces [42].

This behavior is illustrated by figure 4(b) showing partial LDOS at $E = 0.22 \text{ eV}$. There are five different modes at this particular energy. Parts of the modes $C_1, C_2$ in figure 4(a) which are not inside the Dirac cone of the $y$-$z$ face (light gray area in figure 4(a)) are confined to the $x$-$y$ face. Other modes ($C_3, C_4, ...$) belong to both cones (dark gray area in figure 4(a)).
and are distributed along the entire rod perimeter exhibiting a usual resonance structure. No massless Dirac mode is present in this geometry. Similar behavior is observed for V1, V2, ..., modes, but now V1 and V2 spread over the $y-z$ face.

In the case of a rod oriented in the $z$ direction, the Dirac point position is the same for all its faces. As a consequence, no face-specific surface states appear in this case (figure 5). Figure 5(b) shows an increase in LDOS near the edges of the rod, but it does not correspond to any bound edge states, as is evident from figure 5(a). Indeed, all the modes in figure 5(a) are inside the Dirac cone for the $x-z$ (and $y-z$) face and are therefore distributed over all of the surface of the rod. The gap in the surface states is analogous to the one for the rod, oriented in the $y$ direction.

### 3.3. 2D topological insulator state in a thin ribbon

Another question of interest to us is a possibility of appearance of 1D edge states in a thin rod (ribbon) of a topological insulator. Oscillating character of the slab energy gap (see figure 2) indicates periodical energy gap inversion leading to the development of such states. In figure 3 we see two deep gorges along $x$ and $z$ axes, the deepest one for $L_x \approx 6.6$ nm, and the next one for $L_z \approx 3.0$ nm. The gorges relate to the first regions of the gap inversion along respective directions. Gorges corresponding to other inversion regions of thickness are negligible due to much larger decay lengths of the edge states (see below) and have therefore no practical interest.

Figure 6(a) shows the energy structure of a ribbon with the critical thickness $L_x = 6$ nm corresponding to the deepest gorge. 1D edge state with Dirac-like spectrum is clearly seen. Figure 6(b) shows the spacial distribution of LDOS across the sample cross-section. Here the energy corresponds to the Dirac point. Thus, 1D states with Dirac energy spectrum develop near the edges of a thin ribbon in a proper thickness region. So such a ribbon can be considered a 2D topological insulator.

In a ribbon of finite width, hybridization of the 1D edge states results in the energy gap shown in figure 2. Very slow decay of the gap with increase of ribbon width corresponds to $\approx 5$ times larger decay length in comparison with the surface states. In practice, such a slow decay means the properties of the 2D topological insulator can be clearly observed only in relatively large flakes with sizes in the range of tens of nanometers.

### 3.4. Surface step

The most experimentally relevant object is a surface step. Two types of steps are analyzed: low (step height $L_s \lesssim \lambda$) and high ones ($L_s \gg \lambda$).

Figure 7(a) shows energy dispersion curves of a slab hosting high surface steps. The energy spectrum is more complex in
comparison with geometries described above. It demonstrates the same Dirac cone-like mode as a flat surface (figure 1(a)) and quantized states as in a rod (figure 4). The survival of the Dirac cone is a consequence of the absence of the Berry phase contribution in this case, in contrast to the case of the rod. The quantized states are now split in two. The splitting is caused by the difference of surface states dispersion on the top and the side surface of the step.

Figures 7(b)–(l) show partial LDOS obtained for different components of the spectrum below the Dirac point (left set of Figure 7.

Figure 7. (a) Energy dispersion curves for stepped surface (step width 20 nm, step height 10 nm). Each mode is doubly degenerate. Dashed and dash-dotted lines correspond to $E(k_x = 0, k_y)$ and $E(k_y, k_z = 0)$ for $x$–$y$ and $y$–$z$ faces respectively. (b)–(l) Distribution of the partial LDOS for electron states with $E = -0.13$ eV (dashed line in (a)) and $k_y = 0.555 \text{nm}^{-1}$ (b), $0.503 \text{nm}^{-1}$ (c), $0.449 \text{nm}^{-1}$ (d), $0.372 \text{nm}^{-1}$ (e), $0.355 \text{nm}^{-1}$ (f) and for $E = 0.22$ eV (dotted line) and $k = 0.471 \text{nm}^{-1}$ (g), $0.432 \text{nm}^{-1}$ (h), $0.421 \text{nm}^{-1}$ (i), $0.269 \text{nm}^{-1}$ (j), $0.256 \text{nm}^{-1}$ (k).

Figure 8. (a) Energy dispersion curves for stepped surface with low steps (step width 30 nm, step height 2 nm). Each mode is doubly degenerate. Dashed and dash-dotted lines correspond to $E(k_x = 0, k_y)$ and $E(k_y, k_z = 0)$ for $x$–$y$ and $y$–$z$ faces respectively. (b)–(k) Cross-sectional partial LDOS distribution for different modes at electron energies $E = -0.13$ eV (dashed line) in a slab with stepped surface. $k = 0.485 \text{nm}^{-1}$ (b), $0.432 \text{nm}^{-1}$ (c), $0.413 \text{nm}^{-1}$ (d), $0.270 \text{nm}^{-1}$ (e), $0.255 \text{nm}^{-1}$ (f) and for $E = 0.25$ eV (dotted line) and $k = 0.471 \text{nm}^{-1}$ (g), $0.432 \text{nm}^{-1}$ (h), $0.421 \text{nm}^{-1}$ (i), $0.269 \text{nm}^{-1}$ (j), $0.256 \text{nm}^{-1}$ (k).

comparison with geometries described above. It demonstrates the same Dirac cone-like mode as a flat surface (figure 1(a)) and quantized states as in a rod (figure 4). The survival of the Dirac cone is a consequence of the absence of the Berry phase contribution in this case, in contrast to the case of the rod. The quantized states are now split in two. The splitting is caused by the difference of surface states dispersion on the top and the side surface of the step.

Figures 7(b)–(l) show partial LDOS obtained for different components of the spectrum below the Dirac point (left set of
levels at $k_z = 0$. Splitting of surface states is smaller now. However, no quantization along the $z$ direction is observed. The Dirac mode is also present in the spectrum. We also see that there is a mode with the Dirac spectrum, which is non-uniformly spread over the surface.

One of the central questions of the present analysis is the prediction of the model for STS near a step edge. Figure 10 shows LDOS in a thin surface layer as a function of the distance from the step edge taken in the energy intervals around the Dirac point. We see that despite the presence of modes highly localized near the step edges at certain energies (see figure 8(b)), LDOS of the surface layer exhibits only a slight variation ($\lesssim 20\%$) near the step, in agreement with the estimates described in [39]. This result supports also a conclusion of [40] that the main contribution to the increase of LDOS near the step $[39]$ is reproduced by this model. A decrease of LDOS is observed near the concave part of LDOS in a thin surface layer as a function of the surface length $L_{eff} = L_x + 1.8L_z$ for stepped surface with periodical boundary conditions.

Very similar behavior is observed in a slab with low steps (figure 8). The features of LDOS resemble the ones described above for the rod. Namely, there are modes belonging only to a certain face ((b), (c), (g), (h)) as well as modes distributed over all faces. Again as in the case of the rectangular rod the face-specific modes can be identified as the ones lying inside the surface states cone of one face and outside of the surface states cone of the other face (light gray area in figure 7(a)). We also see that there is a mode with the Dirac spectrum, which is non-uniformly spread over the surface.

Figure 9 shows the energy difference between the quantization levels at $k_z = 0$ as a function of inverse effective surface length $1/L_{eff} = 1/L_x + 1.8L_z$ where $L_x$ is the step height. We see that resulting dependence is linear despite very different $L_x/L_s$ proportion, in agreement with equation (3).

4. Summary

We see that the effective continuous model [12] reproduces a number of well-known features of topological insulators, namely the presence of the surface states with the same depth distribution, as ab initio calculations [30], different dispersion laws and Dirac point positions on different crystal faces also known from ab initio calculations [36], oscillatory character of the band structure versus slab thickness [31, 32]. Thus this model can serve as an effective tool for analysis of topological insulator nanostructures. Its convenience is due to a small number of parameters and the possibility to model large nanostructures.

The model predicts a 2D topological insulator state in slabs oriented not only along the $x$ and $y$ but also along the $z$ axis. No edge states localized near the rod’s edges or at the step edge appear in the framework of this model. We find instead modes localized on different faces of the rod running along the $y$ direction. Such states appear also in tight binding calculations [26]. We argue that the modes are massive and their origin is due to the difference in the Dirac point energy of adjacent faces. No such states are found in the rod running along the $z$ direction, as the surface states of its faces have the same Dirac point position.

For the large steps running along the $y$ direction we find modes localized at the top or side surface of the step similar to the case of the rod. The wave functions on the small steps behave in a different manner. The tendency of the modes to localize on one or the other step is counteracted by the tendency of the surface states to spread out, which is made possible by the fact that the step height is smaller than the penetration depth of the surface states. At the same time, the small increase of the LDOS near the step [39] is reproduced by this model. A decrease of LDOS is observed near the concave part.
of the steps. In a real situation the difference in Dirac point position on different surfaces would lead to a potential difference and hence to redistribution of the electron density [51], including possibly formation of bound states [42].

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