Ab-initio transport across Bismuth Selenide surface barriers

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We investigate the effect of potential barriers in the form of step edges on the scattering properties of Bi₂Se₃(111) topological surface states by means of large-scale ab-initio transport simulations. Our results demonstrate the suppression of perfect backscattering, while all other scattering processes, which do not entail a complete spin and momentum reversal, are allowed. Furthermore, we find that the spin of the surface state develops an out of plane component as it traverses the barrier. Our calculations reveal the existence of quasi-bound states in the vicinity of the surface barriers, which appear in the form of an enhanced density of states in the energy window corresponding to the topological state. For double barriers we demonstrate the formation of quantum well states. To complement our first-principles results we construct a two-dimensional low-energy effective model and show that band bending plays a significant role in the scattering process. Our findings are discussed in the context of a number of recent experimental works.

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I. INTRODUCTION

Bismuth selenide has emerged as the prototypical topological insulator material due to a single Dirac cone in the surface band structure and a relatively large bulk band gap. In 2009, concurrent theoretical works revealed the topological insulator phase of Bi₂Se₃. Since then many fundamental properties of topological states have been demonstrated in this material, which has been called the Hydrogen atom of topological insulators.⁹

In recent years, there has been a rapid expansion in the number of scanning tunneling microscope (STM) experiments on the Bi₂Se₃(111) and the closely related Bi₂Te₃(111) surface. Impurities on bismuth selenide have been imaged and scattering mediated by bulk states has been observed.³⁵ Additionally there have been studies of dopants on the bismuth telluride surface⁹ and, interestingly, a bound state at a surface step of Bi₂Te₃ has also been found.¹¹ On the theoretical front, there have been several efforts towards modeling scattering of these surface states from perturbation theory by employing Dirac-like model Hamiltonians and by imposing symmetry considerations.¹²¹³ Furthermore, a study of robustness of surface states against on-site disorder by employing first-principles calculations was also reported.¹⁵

In this paper, we investigate the effect of step barriers at the Bi₂Se₃(111) surface on the scattering properties of the topological states by means of ab-initio transport calculations. We find that, due to the spin-polarized helical nature of the surface band, there is no scattering for normal incidence, since a reflection would entail a 180° backscattering. However, as one moves to non-normal incidence, scattering is revealed. This is because the spins of the counter-propagating channels are no longer antiparallel. An analysis of the local density of states reveals that the surface barrier strongly affects the spin of the surface state, in particular allowing an out of plane spin component, which is negligible in the absence of the barrier. In order to rationalize our ab-initio results we have constructed a potential barrier model based on a simple Dirac Hamiltonian for the surface states. This is solved per barrier of various shapes and a comparison is made with our first-principles calculations. We note in passing that, although our ab-initio calculations have been performed for the particular case of bismuth selenide, we expect the same qualitative results to also hold for step edges perpendicular to directions without hexagonal warping in Bi₂Te₃ and for other related materials like Bi₂Te₃S and TlBiSe₂.

Following this introduction, the remaining of the paper is organized as follows. We begin by describing our computational methods, in particular we outline the procedure for performing the transport calculations. We then study scattering originating from a single surface barrier by analyzing the transmission and the densities of states. Intriguingly our calculations reveal a bound state in the vicinity of the barrier. From there, we move on to construct a low-energy model for the scattering problem, with barrier strength and width extracted from our ab-initio results. Next we look at the analogous problem in the presence of double barriers of different lengths. Notably, we find an energy splitting of the bound state when the states at the two barriers interact directly as in the case of a short double barrier, as well as when the bound states couple with quantum well states formed in the case of a longer double barrier. Finally we summarize our results and conclude.

II. COMPUTATIONAL METHODS

Our transport calculations have been performed by using the Smeagol code, which combines the density functional theory (DFT) numerical implementation contained in the Siesta code with the non-equilibrium Green’s function method for electron transport. Here we briefly outline the calculation procedure and refer the readers...
structure along the transport direction, spheres represent Selenium and Bismuth atoms, respectively. The yellow and purple

FIG. 1: (Color online) (a) The unit cell of the 3-QL slab leads used in the transport calculations. The yellow and purple

 bulk system. The transport calculation proceeds by using an equivalent infinite algorithm is calculated by using an equivalent infinite

case is a surface step. The Hamiltonian needed for the

self-energies of the leads are denoted by $f_\alpha$ and $\Gamma_\alpha = (\Sigma_\alpha - \Sigma_\alpha^L)$ are the broadening matrices. In order to perform the contour integral in Eq. (2) we use 16 energy points in the complex semicircle, 16 points along the line parallel to the real axis and 16 poles. The density matrix calculated in Eq. (2) is used by SIESTA to re-evaluate the Kohn-Sham Hamiltonian, and such a procedure is iterated until self-consistency is obtained. Once convergence is achieved, the relevant quantities like the transmission function, $T(E)$, and the density of state (DOS), $N(E)$, are calculated,

$$T(E) = \text{Tr} [\Gamma_R G \Gamma_L G^\dagger], \quad N(E) = \frac{1}{2\pi} \text{Tr} [A(E) S],$$

where $\text{Tr}$ stands for the trace, $A(E) = i(G - G^\dagger)$ is the spectral function and $S$ is the overlap matrix.

In all calculations spin-orbit interaction is included by means of an on-site approximation\cite{22} and the Perdew-Burke-Ernzerhof generalized gradient approximation (GGA) to the exchange-correlation functional is employed. We have used a double-$\zeta$ polarized basis set and a real space mesh cutoff of 300 Ryd. For slab calculations a minimum of 25 Å vacuum region has been included to prevent spurious interaction between periodic replicas. We use $3 \times 1 \times 1$ $k$-point mesh to obtain the self-consistent potential (here $x$ is the direction perpendicular to the transport direction in the plane of the slab, $y$ is along the slab height and $z$ is the transport direction). When calculating the integrated transmission and DOS we use 101 $k$-points along the $x$ direction. Periodic boundary conditions have been considered in the plane orthogonal to the transport direction, while using open boundary conditions along the transport direction allows us to simulate a single scatterer, which, in this particular case is a surface step.

The unit cell used for the leads is shown in Fig. 1(a). It consists of a three quintuple-layers (3-QL) thick slab terminated on both sides by Se atoms, as found experimentally. For the slab we use the experimental lattice constants. The corresponding band structure is shown in Fig. 1(b). Note that there is band folding as a consequence of the doubling of the Bi$_3$Se$_3$ primitive unit cell. The bandstructure reveals the Dirac cone and the helical states consistent with earlier studies.\cite{10} It should also be

direct inversion

$$G(E) = [E + i0^+ - H - \Sigma_L - \Sigma_R]^{-1},$$

where $\Sigma_\alpha$ is the self-energy of the left-hand side ($\alpha=L$) and right-hand side ($\alpha=R$) lead. The charge density is then calculated by integrating the non-equilibrium Green’s function along a contour in the complex energy plane

$$\rho(E) = \frac{1}{2\pi} \int dE G^<(E),$$

where $G^<(E) = iG[f_\alpha \Gamma_L + f_R \Gamma_R]G^\dagger$ is the lesser Green’s function for the transport problem. The Fermi functions for the leads are denoted by $f_\alpha$ and $\Gamma_\alpha = (\Sigma_\alpha - \Sigma_\alpha^L)$ are the broadening matrices. In order to perform the contour integral in Eq. (2) we use 16 energy points in the complex semicircle, 16 points along the line parallel to the real axis and 16 poles. The density matrix calculated in Eq. (2) is used by SIESTA to re-evaluate the Kohn-Sham Hamiltonian, and such a procedure is iterated until self-consistency is obtained. Once convergence is achieved, the relevant quantities like the transmission function, $T(E)$, and the density of state (DOS), $N(E)$, are calculated,

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direction. Different curves correspond to different components of the wave-vector, orthogonal to the transport barrier setup. We investigate two barrier lengths, where half the length of the scattering region. For the double barrier case the 4-QL region extends over about the step extends over a region of 49.72 Å in the shorter case and is 149.16 Å for the longer one. Note that such large cells require an accurate order-N algorithm as the one available in SMEAGOL. 

III. SCATTERING FROM A SINGLE BARRIER

We begin our analysis by looking at the transport across a single surface barrier [see Fig. 1(a)], for which the transmission function is shown in Fig. 2(a) as a function of energy and for different values of the component of the wave-vector. At normal incidence \((k_x = 0)\), the surface states are perfectly transmitted, \(T = 2\), due to their helicity. As such, our first-principles calculations confirm Klein tunneling. The transmission of bulk states, however, is reduced by the presence of the step edge. In contrast, as soon as one moves away from normal incidence, the transmission is no longer integer-valued. In particular, it dips below \(T = 2\), indicating substantial scattering. Fig. 2(b) shows the total transmission obtained by integrating \(T(E, k_x)\) over all angles of incidence, namely \(T_{\text{total}} = \frac{1}{\Omega_{\text{BZ}}} \int_{k_x} T(E, k_x) dk_x\), where \(\Omega_{\text{BZ}}\) is the length of the Brillouin zone. Notably, \(T_{\text{total}}\) retains the characteristic “V-shape” associated with the linear Dirac cone-like bands, despite the presence of the barrier. Overall we can conclude that the total transmission in presence of the barrier is quite close to the one for the unperturbed slab [compare the red and black curve in Fig. 2(c)].

At non-normal incidence the spin projections of the surface states counter-propagating at a given edge are no longer anti-parallel and thus backscattering becomes allowed, even in the absence of a perturbation that breaks time-reversal symmetry. The situation is schematically illustrated in Fig. 2(d), and its consequences are demonstrated in Fig. 2(c), where we plot the transmission across the surface barrier as a function of \(k_x\) at different energies. Clearly \(T(E, k_x)\) is reduced as \(k_x\) increases, which is expected from argument related to the spin projections of the two counter-propagating surface states. At large incidence angles the transmission tends towards the residual value of one, since a perfectly transmitted surface state is present at the opposite side of the slab (no scattering center is present on the opposite surface). It can be shown that the maximum scattering amplitude is proportional to \(\frac{1}{2}(1 + \cos \theta)\), where \(\theta\) is the angle between the spin directions of the surface states. Note that at higher energies, the transmission persists at values around the unperturbed one, \(T = 2\), for larger incidence angles. This is because as one moves the Fermi level at higher energy, the Fermi circle gets larger. As a consequence the same \(k_x\) corresponds to an angle of incidence closer to the direction normal to the step edge.

![FIG. 2: (Color online) (a) Transmission across the surface barrier as a function of energy at different values of \(k_x\) component of the wave-vector, orthogonal to the transport direction. Different curves correspond to different \(k_x\) starting from \(k_x = 0\) up to \(k_x = 0.03475\) Å\(^{-1}\), in equal steps of 0.002317 Å\(^{-1}\). Note the perfect transmission at \(k_x = 0\). At other incidence angles \(T\) is reduced. (b) The total transmission integrated over \(k_x\) in the presence (black curve) and absence (red curve) of the barrier. (c) The transmission as a function of \(k_x\), at different constant energy cuts in the energy region of the surface states. Note that \(T\) is reduced from \(T = 2\) at non-zero angle of incidence and with sufficiently large \(k_x\) drops down towards \(T = 1\). Non-zero reflection at the barrier can be explained using the schematic diagram shown in (d). At non-normal incidence there is a finite overlap between the spin projections of the forward and backward moving surface state. Backscattering at angles away from normal incidence is present even in the absence of time-reversal symmetry breaking perturbations.](image-url)
FIG. 3: (Color online) The DOS projected on the surface atoms along the scattering region at (a) $k_x = 0$, (b) $k_x = 0.032$ Å$^{-1}$ and (c) integrated over all $k_x$. At $k_x = 0$ there are no oscillations. These start to emerge at $k_x = 0.032$ Å$^{-1}$ but are not visible in the average. Note in all figures an enhanced DOS on the left-hand side of the barrier. The second column of panels show the Fourier transform of the projected DOS in the flat region adjacent to the barrier, at the corresponding $k_x$. The scattering vector resulting from backscattering at non-normal incidence is clearly seen in (b). The average, however, reveals no scattering. Here and henceforth warmer colors represent higher and cooler colors indicate lower values, respectively. The third column shows the transmission as a function of energy for the three cases. For $k_x = 0$ and $k_x = 0.032$ Å$^{-1}$, we also plot the band structure along transport direction for comparison.

In PDOS are seen after reflection from the step edge. However, moving away from normal incidence, the above-mentioned oscillations begin to appear. By analyzing the PDOS of the atoms at the bottom surface we have checked that such scattering occurs only at the top one, i.e., it is caused by the presence of the step edge. The scattering vectors can be obtained by performing a Fourier transform of the DOS along the long flat region adjacent to the barrier. At $k_x = 0$, expect-edly there are no prominent scattering processes. As one moves to $k_x = 0.032$ Å$^{-1}$, there appears a dominant scattering wave-vector in the Fourier transform starting at 0.1 eV and extending upwards in energy, as shown in Fig. 3(b). This corresponds to backscattering at a non-normal incidence angle. Furthermore, this can be mapped to band structure along the transport direction, where a band starting at the same energy is present. The average over $k_x$, however, reveals no scattering on this scale, even though there is a clear back scattering at individual $k_x$. In order to accurately resolve the small density oscillations above the average, one would need to consider many more $k_x$-points in the calculation. This is computationally prohibitively expensive for the system sizes considered here, and a more detailed investigation of the oscillations will be reported elsewhere. For all three cases we also plot the transmission as a function of energy, for comparison with the surface PDOS.

Fig. 3 also makes apparent the band bending (of the order of 0.04 eV) introduced by the step. This has also been observed experimentally in samples with cleaved...
FIG. 4: (Color online) The spin-resolved local density of states for states incoming from the left-hand side lead with an energy 0.175 eV above the Fermi level. We plot the spin projection along the (a) $x$, (b) $y$ and (c) $z$ direction at $k_x = 0$. On the right-hand side (d), (e) and (f) are the corresponding plots for $k_x = 0.032 \, \text{Å}^{-1}$. Here red color represents positive values while blue stands for negative ones. Scattering at the step edge even at $k_x = 0$ allows the spin to rotate out of the plane of the slab resulting in finite $y$ and $z$ components, in contrast to the unperturbed bottom surface where these are negligible. At non-normal incidence ($k_x = 0.032 \, \text{Å}^{-1}$) the $z$ component of the spin-resolved LDOS becomes finite, while the step edge introduces a non-zero $y$ component. The insets are zooms around the step edge.

IV. A LOW-ENERGY MODEL

In order to interpret our ab-initio results we construct a simple potential barrier model for the scattering problem. The surface states are described by a Dirac Hamiltonian

$$
\mathcal{H} = e_0 \sigma_2 \times \sigma_2 + \begin{pmatrix}
V(z) & v(k_z - i k_x) \\
v(k_z + i k_x) & V(z)
\end{pmatrix},
$$

where $e_0$ is the energy of the incoming states, $\sigma$ are the Pauli matrices, $V$ is the potential barrier, and $v$ is the velocity of the incoming states. These equations capture the essential physics of the scattering process at the step edge.
where the potential profile $V(z)$ is shown in Fig. 5(a). The values of $\epsilon_0 = -0.05$ eV and $v = 4.58$ eVÅ, are obtained from our first-principles band structure. Here we consider only the upper part of the cone, i.e., $E = V(z) + \sqrt{k_x^2 + k_z^2}$. The corresponding eigenstate is given by,

$$\psi(k_x, k_z) = \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{k_x^2 + k_z^2}} \right) e^{i\mathbf{k} \cdot \mathbf{r}}. \quad (5)$$

One can then use the wave-function continuity conditions at the potential steps to solve for the transmission and reflection coefficients in a straightforward manner. The potentials in the 4-QL and 3-QL leads, respectively $V_1$ and $V_4$, are nearly identical and are set to zero. $V_2$ is the potential associated to the barrier and extends over a length $d$, while $V_3$ is the band bending, which is finite over a distance $L$. The calculated transmission curves are plotted in Fig. 5(b) for $V_3 = -0.02$ eV and in Fig. 5(c) for $V_3 = 0$. The shape of transmission is much closer to that obtained from the ab-initio calculations for finite $V_3$, as compared to the situation where $V_3 = 0$. This suggests that band bending plays an important role in the scattering from step edges and should be taken into consideration. We note that this simple model does not take into account the three-dimensional nature of the scattering problem as well as it neglects the change in spin orientation of the surface states near the barrier. Despite these deficiencies the model can qualitatively reproduce the transmission obtained from first-principles, although only an atomistic description is capable of describing the fine details of the scattering process. We note that several models have been proposed to study topological states on a curved surface. These predict no backscattering at any angle from hyperbolic steps. Unfortunately these models are not valid for atomic-scale abrupt steps that we have studied in this work.

V. SCATTERING FROM DOUBLE BARRIERS

We now analyze the scattering properties of double barrier structures constructed over the Bi$_2$Se$_3$(111) sur-
FIG. 7: (Color online) DOS projected on the surface atoms along the double barrier scattering region at (a) $k_x = 0$, (b) $k_x = 0.032$ Å$^{-1}$ and (c) integrated over all $k_x$. Note the absence of density oscillations for $k_x = 0$ and for the integrated DOS. Incidence at finite $k_x$ leads to density oscillations clearly seen in the long flat region adjacent to the barrier as shown in (b). The panels on the right-hand side are the corresponding Fourier transforms, which are featureless for (a) and (c), while scattering is clearly present in (b).

FIG. 8: (Color online) PDOS on the surface atoms for a double barrier of length 149.16 Å at (a) $k_x = 0$ and (b) $k_x = 0.032$ Å$^{-1}$. Note the absence of quantum well states in (a). In (b) quantum well states interact with the bound state at the two barriers leading to energy splitting of the bound state.

The $k_x$-resolved and total DOS projected on the surface atoms is plotted in Fig. [7], where the bound state can be clearly seen in the 4-QL region extending from 10 Å to 60 Å. The DOS associated to such bound state oscillates and decays towards the center of the quantum well defined by the two barriers at the step edges. A band bending similar to that observed for the single barrier is also seen for this particular barrier configuration. The interaction between the bound states localised at the two barriers splits them in energy, creating alternating high and low DOS as one moves up along the energy axis. Another noticeable feature is a state localized in the 4-QL region at around 0.1 eV [see Fig. [7(b)]]. This is an additional state in the 4-QL slab, which is decoupled from the 3-QL leads. The same state is absent in the case of a single barrier produced by a step edge between a 3-QL and a 4-QL semi-infinite lead. The Fourier transforms of potential barriers. In Fig. [8(b)] we plot the transmission as a function of the incident $k_x$ for different energies. Away from the resonances the transmission shows again a cosine-like behavior with transmission going down to $T = 1$ as the incidence angle increases ($k_x$ gets larger).
the DOS display similar features as those shown in Fig. 3. However, in the double barrier case the resolution is improved over that of the single barrier structure since we now have more atoms along the flat region next to the barrier.

Note that for this particular chosen length of the double barrier there are no quantum well states formed inside the 4-QL region. However, for a longer barrier the quantum well states appear, as demonstrated by the PDOS on the surface atoms at two different $k_x$ for a barrier of length 149.16 Å [see Fig. 8]. At normal incidence no quantum well states can be formed in the energy window of the surface state, since the two surface states have opposite spin projections leading to no interference. In contrast, at finite $k_x$ quantum well states appear (e.g. a nodeless state at around 0.13 eV and a single-node state at around 0.16 eV). However, the behavior of these states near the edges of the barrier is different from usual because of the presence of the bound state. In fact, these quantum well states interact with the bound states at the edges of the barrier resulting in an energy splitting of the bound state. We observe splitting of the bound states in both the short and the long double barrier, in the former case due to the interaction between the bound states located at the two edges of the 4-QL region, while in the latter due to the bound state interacting with the quantum well state within the barrier.

VI. SUMMARY

We have used ab-initio transport theory to study scattering to both single and double barriers of the topologically protected states present on a Bi$_2$Se$_3$(111) surface. In particular we have studied the dependence of the transmission on the angle of incidence and the electron energy. At normal incidence our first principles approach confirms Klein tunneling. Furthermore, we have calculated the density of states projected on the surface atoms and found bound states localised only on the higher side of the barrier. Thus our local density of states plots make apparent the three-dimensional nature of the scattering problem, in which the spins of the surface states are no longer confined to the plane of the topological insulator slab. We have also constructed a simplified potential barrier model using linear Dirac bands to compare with our first principles calculations. Throughout the paper we have placed our results in the context of recent experimental works.

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