Topological insulator “nanotubes”

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Abstract. Low-energy electronic states in a topological insulator nanowire is studied theoretically. We highlight the role of spin Berry phase which distinguishes transport characteristics of such a nanowire from those of a single-wall carbon nanotube.

1. Introduction

Topological insulator nanowire resembles a stuffed carbon nanotube. The topological insulator has a seemingly contradictory property of being metallic on its interface, albeit insulating in the bulk. Motivated by a recent Aharonov-Bohm measurement on a topological insulator nanowire, [1] we investigate electronic states on the surface of a long cylinder filled with a topological insulator compound such as Bi\(_2\)Se\(_3\), Bi\(_2\)Te\(_3\), etc. Since inside of the cylinder the spectrum is gapped, the transport characteristic of such a nanowire is comparable to that of a single-wall carbon nanotube (Fig. 1). However, as we reveal in this paper, the existence/absence of spin Berry phase [2] brings a crucial difference between the two systems.

2. Bulk-surface correspondence: derivation of the spin Berry phase

Let us start with the following simple effective Hamiltonian for bulk 3D topological insulator, [3, 4, 5]

\[
H = \begin{bmatrix}
M & Ak_z & 0 & Ak_- \\
Ak_z & -M & Ak_- & 0 \\
0 & AK_+ & M & -Ak_z \\
Ak_+ & 0 & -Ak_z & -M \\
\end{bmatrix}
\]  

Figure 1. The topological insulator “nanotube” (left), the topological insulator nanowire (central), and a (bulk) topological insulator pierced by a cylindrical aperture (right).
where \( M = M_0 + M_2(k_x^2 + k_y^2 + k_z^2) \), and \( A \) is a constant. We then consider a situation that a bulk insulating state is confined inside a cylinder of a radius \( R: \sqrt{x^2+y^2} \leq R \), directed, say, along the \( z \)-direction. To identify the gapless surface states in the cylindrical geometry, we decompose, Eq. (1) into two parts:

\[
H = H_{\perp}(k_r) + H_{\parallel}(k_\phi, k_z),
\]

using the cylindrical coordinates: \( x = r \cos \theta, y = r \sin \theta \). To derive the surface effective Hamiltonian we first need to identify suitable basis eigenstates. For that we first consider solving the the eigenvalue equation, \( H_{\perp}|\psi\rangle = E_{\perp}|\psi\rangle \), with the boundary condition of \( (x|\psi\rangle)_{r=R=0} = 0 \). Here, assuming the nanowire geometry (the central image of Fig. 1), we consider solutions of the form, \( (x|\psi\rangle) \sim e^{i\lambda(r-R)} \), \([6, 7, 4, 5]\) which is localized on the inner surface of the cylinder; \( \lambda = ik_r > 0 \), and \( k_r = \sqrt{k_x^2 + k_y^2} \). The solution to this boundary problem is, \(^1\)

\[
|\psi\rangle = \left\{a|\hat{r}+\rangle + b|\hat{r}-\rangle \right\}\left\{e^{\lambda(r-R)} - e^{-\lambda(r-R)}\right\},
\]

where

\[
|\hat{r}+\rangle = \frac{1}{2} \left[ \begin{array}{c} 1 \\ i e^{i\theta} \\ i e^{i\theta} \end{array} \right],

|\hat{r}-\rangle = \frac{1}{2} \left[ \begin{array}{c} 1 \\ -i \\ -e^{i\theta} \end{array} \right].
\]

The effective 2D surface Hamiltonian \( H_{2D} \) is obtained by calculating the matrix elements: \( \langle\langle \pm |H_{\parallel}|\pm \rangle\rangle \), as

\[
H_{2D} = \left[ \begin{array}{cc} 0 & -iBk_z + \frac{A}{R} \left(-i \frac{\partial}{\partial \phi} + \frac{1}{2}\right) \\ iBk_z + \frac{A}{R} \left(-i \frac{\partial}{\partial \phi} + \frac{1}{2}\right) & 0 \end{array} \right],
\]

Factor 1/2 in the off-diagonal elements is the manifestation of the spin Berry phase. The eigenstate of \( H_{2D} \), satisfying

\[
H_{2D} \left[ \begin{array}{c} a \\ b \end{array} \right] = E_{\parallel} \left[ \begin{array}{c} a \\ b \end{array} \right],
\]

has a non-trivial winding property with respect to the rotation of \( \theta \).

3. Finite-size energy gap
The spin Berry phase appearing in the surface Dirac Hamiltonian; cf. Eq. (5), is often discussed in the context of Aharonov-Bohm experiment on topological insulator nanowires. Here, in order to implement a mathematically equivalent situation, we rather consider “bulk” pierced by a cylindrical aperture (the right image of Fig. 1). \([8]\) Topological distinction does not tell which side is vacuum and which side is filled with a topological insulator. Introduction of an aperture in the \( z \)-direction breaks the translational symmetry in the \( (x, y) \)-plane, but leaves the same invariance in the \( z \)-direction. Thus, in the numerical analyses we describe below, we will focus on the spectrum \( E = E(k_z) \). The first panel of Fig. 2 shows that the spectrum of such a punctured topological insulator is gapped. This is a rather unexpected phenomenon, if one recalls that carbon nanotubes become either metallic or semiconducting depending on the way a graphene is rolled up into a tube. \([10]\) Here, a crucial difference from the carbon nanotube case is that the Dirac cone involves a real spin and not a sub-lattice pseudo-spin. The procedure of rolling up a flat surface into a tube introduces a \( 2\pi \)-rotation in spin space along a contour

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Figure 2. Energy spectrum $E(k_z)$ in the presence of a pair of screw dislocations with Burgers vector, $\vec{b} = (0, 0, \pm b)$ where $b = 0$ (upper left), $b = 1$ (upper right), $b = 2$ (lower). $A = 1$. $N_x \times N_y = 16 \times 16$.

winding around the tube once. [2, 8] The resulting $-1$ factor changes the boundary condition around the tube from periodic to anti-periodic:

$$e^{i(p_x + k_{(0)}^z)s} \times (-1) = 1.$$  (7)

The $-1$ factor is also a direct consequence of the spin Berry phase, which combined with the finite size of the cylinder, plays the role of opening a gap in the spectrum (see the upper left panel of Fig. 2). Here, we have decomposed the total crystal momentum of an electron into short- and long-wavelength components: $\vec{k} = k_{(0)}^z + \vec{p}$. $\vec{p} = (p_x, p_y)$ refers to the long-wavelength component measured from the Dirac point. The short-wavelength component $k_{(0)}^z = (k_{(0)}^x, k_{(0)}^y)$ is, on the other hand, a crystal momentum at the Dirac point, and typically $k_{(0)}^z = 0, \pi$. Since the circumference $s = 2N_c$ of the cut is, by its construction, an even integer multiple of the lattice constant, $e^{ik_{(0)}^z s} = 1$ always holds. As a result, the anti-periodicity of the boundary condition (7) must be taken care of solely by the long-wavelength part of the crystal momentum, and eliminates, as seen e.g. in the spectrum of Fig. 2 (upper panel), states on the line $p_x = 0$ crossing the very bottom of a Dirac cone. Low-energy states in the same figure consist of $p_x = \pm \pi/s$, leading to occurrence of a finite-size gap, $\Delta E = 2A\pi/s$, in the spectrum.

4. Protected helical modes along a dislocation line

We then introduce a screw dislocation along the aperture, in order to mimic the flux effect of half a flux penetrating inside of a topological insulator nanowire. Such a lattice scale deformation modifies the periodicity of the wave function associated with the short-wavelength component of the crystal momentum, i.e., $k_{(0)}^z = \pi$ in the present case. The entire effect of a screw dislocation on the electronic wave function is to add a phase shift $e^{ik_zb}$ each time an electron winds around the dislocation line. With this taken into account, the boundary condition modifies as,

$$e^{ip_x s} \times e^{ik_{(0)}^z b} \times (-1) = 1.$$  (8)
Notice that only the part of spectrum associated with the Dirac cone at \((k_z, k_x) = (\pi, 0)\) is sensitive to the dislocation. When \(b\) is an odd integer, \(p_x = 0\) state is now allowed, and the spectrum becomes gapless at \(k_z = \pi\). When \(b\) is an odd (even) integer, the \(p_x = 0\) state is now allowed (remains forbidden), and the spectrum becomes gapless (remains gapped) at \(k_z = \pi\).

Such even/odd (gapped, gapless, gapped, · · ·) feature has been fully confirmed in our numerical simulations depicted in Figs. 2. In terms of the Aharonov-Bohm experiment, the existence of dislocation lines with \(b = 1, 2, 3, \cdots\) corresponds to a nanowire example penetrated by a flux \(\phi = \pi, 2\pi, 3\pi, \cdots\).

5. Further comments on numerical simulations

To implement the Hamiltonian (1) on a square lattice as a tight-binding model, we replace the \(k\)'s in Eq. (1) by \(\sin k\)'s and \(k^2\)'s in \(M\) by \(2(1 - \cos k)\)'s. We also consider a case of \(M_0\) taking a large absolute value, \(M_0/M_2 = -6\), since the screw dislocation can mimic a magnetic flux only for Dirac cones located at a finite (but still a time-reversal invariant) crystal momentum. In the example we have further examined \((M_0/M_2 = -6)\) the bulk system is a weak topological insulator, and therefore bears an even number of (usually two) gapless Dirac cones on its surface.

For example, on the surface perpendicular to the \(y\)-axis (i.e., \((z, x)\)-plane, for instance) these two Dirac cones are located at \((k_z, k_x) = (0, \pi)\) and \((k_z, k_x) = (\pi, 0)\).

In three panels of FIG. 2 one can recognize remnants of these two Dirac cones projected onto the \(k_z\)-axis (i.e., in the band structure in the vicinity of \(k_z = 0\) and \(k_z = \pi\)). On the top panel, both of these remnants of Dirac cones are gapped due to a finite size of the aperture (here, the circumference \(s\) of the aperture is twice the cut width; \(s = 2N_v\)). Notice at this point that the dislocation acts only on the ”Dirac cone” at \(k_z = \pi\) as a flux. When the magnitude of dislocation \(b\) is an odd integer, this effect compensates the spin Berry phase \(\pi\) and closes the gap at \(k_z = \pi\).

6. Conclusions

Using a simple model for a topological insulator implemented on a square lattice, we have systematically studied the nature of electronic states on curved surfaces. Taking, as an example, the case of a weak topological insulator, we have contrasted the stability of 1D gapless helical modes and the non-robustness of (even number) 2D surface Dirac cones. Comparing the case of a topological insulator nanowire threaded by a magnetic flux and of a bulk topological insulator punctured and distorted by a dislocation line, we have highlighted the role of spin Berry phase in transport characteristics. The proposed scenario is closely related to the mechanism of recently observed anomalous Aharonov-Bohm oscillations in a topological insulator “nanotube”.

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