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Effects of an external electric field on electronic states and transport of a Bi_2Se_3 thin film

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ABSTRACT

We study the electronic band structure, density distribution, and electronic transport of surface states in a Bi_2Se_3 thin film. By using the four-band model, it is demonstrated that an appropriate external electric field can eliminate the coupling between the top and bottom surface states of the film, and contribute to the realization of the quantum spin Hall effects. However, a sufficient high electric field may destroy the property of the surface states. Using the scattering matrix approach, we further study theoretically the spin-dependent electron transport of a Bi_2Se_3 thin-film junction. Interestingly, a transverse electric field can switch on/off the spin-up or -down electronic channel of the surface states in the junction.

1. Introduction

A topological insulator (TI) is a new quantum substance state, originating from spin-orbit coupling (SOC), characterized by a full insulating gap in the bulk and gapless surface/edge states protected by time-reversal symmetry [1–3]. TIs exhibit many new quantum effects and electromagnetic features [4,5], and may be extensively used in spintronic devices with high speed and low consumption as well as quantum information processing. Among all known three-dimensional (3D) TIs, bismuth selenide (Bi_2Se_3) possesses of a large band gap (∼0.3 eV) for bulk and a single Dirac cone in the gap for surface states [6,7], which were confirmed in photoemission experiments [8]. While, the transport properties of surface states are difficult to observe in experiments since the surface contribution is often masked by the conductivity of impurities or defects in the bulk [9–14]. In 3D TI thin films, however, the bulk contribution is greatly suppressed, which renders the peculiar transport properties of surface states easier to be observed. Thanks to the up-to-date semiconductor technologies, high-quality Bi_2Se_3 thin films [15] and nanoribbons have been fabricated [16]. This has stimulated many theoretical works on the thin films of 3D TIs [17,19,18]. With the decrease of the thin films thickness, the surface states on the top and bottom surfaces couple each other [17], and alternate between topologically trivial and nontrivial two-dimensional (2D) behavior [19]. Therefore, applicable methods are needed to eliminate the coupling between the top and bottom surface states of the film.

The Datta-Das spin-transistor [20], actually, is a spin filter, where the spin of charges is modulated electrically by a gate-dependent Rashba SOC in a semiconductor heterostructure connected to two ferromagnetic electrodes [21]. However, it is demonstrated that the spin-transistor is difficult to be realized due to the spin relaxation in the system and the interfacial effects between different materials [22]. Fortunately, TIs appear to be promising candidates for spintronic devices because of topological materials with strong SOC which leads to the formation of spin-momentum locked Dirac fermions at the edges or surfaces. In addition, TIs possess many novel transport properties, such as helical edge states or surface states [23,6,7], suppression of backscattering [24,26,25], etc. In particular, the electrical control of spin-dependent transport is an interesting issue in TIs, it has attracted much attention in recent years [27–33]. Due to the finite size effects, the edge states couple to each other in a narrow HgTe/CdTe Hall Bar. Taking into account the weak disorder or interaction scattering, electron scattering between the edge states becomes possible. But, applying an external electric field, the edge channels in the narrow HgTe/CdTe Hall bar can be switched on/off, and realize to/destroy quantum spin Hall effect [30,34].

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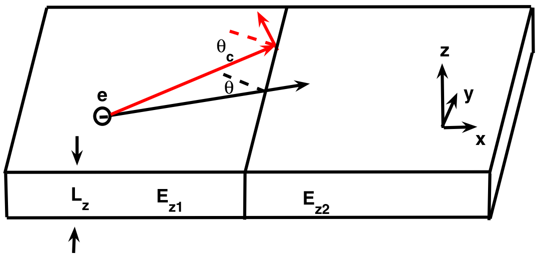

Fig. 1. Schematic structure of a Bi_2Se_3-thin-film junction between regions with different electric fields which are perpendicular to the surface, one of them $E_{z1} = 1.2 \times 10^5$ along $-z$ direction, separating the spin-up and -down surface states from each other. E_{z2} is adjustable, controls the transport of the system.

In this work, we firstly investigated the electron band structure and electronic density distribution of surface states in Bi_2Se_3 thin films. We demonstrated that an appropriate electric field can eliminate the coupling between top and bottom surface states of the films, separate the spin-up and spin-down surface states. But, a high electric field may destroy the topological properties of surface states in the film. Secondly, we studied theoretically spin-dependent transport of surface states in a Bi_2Se_3 thin-film junction with two transverse electric fields E_{z1} and E_{z2} which are perpendicular to the plane of the Bi_2Se_3 thin film (see Fig. 1). One of them E_{z1} separates the spin-up and -down surface states from each other at the left side of the junction. The other E_{z2} controls the electron transport at the right side of the junction. We will show that the transverse electric fields can switch on/off the spin-up (or spin-down) electronic channel of surface states. Our results may provide a simple way for the design of potential application of spintronic devices.

The paper is organized as follows. In Sec. 2, we introduce the Hamiltonian of the system, consider the spin dependent transport of surface states, and present its analytical solutions. The results and discussions are arranged in Sec. 3. The conclusion is given in Sec. 4.

2. Model and formulism

In the analysis, we use an effective four-band model [6] which describes the low-energy physics of 3D TI materials like Bi_2Se_3 or Bi_2Te_3 centered around the Γ point in the Brillouin zone. In the basis states $\{P1_z^+,\uparrow\rangle, P2_z^-,\uparrow\rangle, P1_z^+,\downarrow\rangle, P2_z^-,\downarrow\rangle\}$, the low-energy Hamiltonian reads

$$H_{3D} = \begin{bmatrix} \epsilon_k + M(k) & -iA_1\partial_z & 0 & A_2k_- \\ -iA_1\partial_z & \epsilon_k - M(k) & A_2k_- & 0 \\ 0 & A_2k_+ & \epsilon_k + M(k) & iA_1\partial_z \\ A_2k_+ & 0 & iA_1\partial_z & \epsilon_k - M(k) \end{bmatrix}, \quad (1)$$

where $\epsilon_k = C - D_1\partial_z^2 + D_2(k_x^2+k_y^2)$, $M(k) = M + B_1\partial_z^2 - B_2(k_x^2+k_y^2)$, and $k_\pm = k_x \pm ik_y$. The material parameters C, D_1, D_2, M, B_1 and B_2 are usually determined from first-principles calculation [6]. In the presence of an external electric field, the total Hamiltonian is written as

$$H = H_{3D} + V(z), \quad (2)$$

where $V(z) = q\epsilon_0/(\epsilon_0 + \epsilon_r)\vec{E}_z \cdot \vec{z}$ is the potential induced by an external electric field $\vec{E}_z$ along the z direction, q is the electric charge of an electron, $\epsilon_0 = 1$ for air environment, ϵ_r is the dielectric constant, and $\epsilon_r = 113$ for the film. For this quasi-2D system, the single-electron envelope function is given as follow:

$$\psi(x,y,z) = e^{i\vec{k}\cdot\vec{r}} \sum_n \alpha_n \varphi_n(z), \quad (3)$$

where α_n is a 4×1 matrix, $\varphi_n(z) = \sqrt{\frac{2}{L_z}} \sin\frac{n\pi}{L_z}(z + \frac{L_z}{2})$, L_z is the thickness of the Bi_2Se_3 film, and $n = 1, 2 \cdots j$. The number of terms j in the summing series should be large enough to obtain a convergent numerical result. Using the above envelope function, the matrix elements of Hamiltonian (2) can be derived. Consequently, the band structure, the wave functions and the density distributions of the films can be numerically obtained.

Next, we consider the electron tunneling through the junction (as shown in Fig. 1). The wave functions in the junction between left (L) and right (R) sides can be expressed as

$$\psi^L(x \le 0) = \sum_n [e^{ik_n^L x\cos(\theta_n^L)} \sum_j \alpha_{n,j}^L \varphi_j^L(z) + \sum_m r_{mn} e^{-ik_m^L x\cos(\theta_m^L)} \sum_j \alpha_{m,j}^L \varphi_j^L(z)] e^{ik_n^L y\sin(\theta_n^L)}, \quad (4)$$

and

$$\psi^R(x \ge 0) = \sum_{n',n} [t_{n'n} e^{ik_{n'}^R x\cos(\theta_{n'}^R)} \sum_j \alpha_{n',j}^R \varphi_j^R(z)] e^{ik_{n'}^R y\sin(\theta_{n'}^R)}, \quad (5)$$

where the angles $\theta_n^L = arctan(k_{y,n}^L/k_{x,n}^L)$ and $\theta_{n'}^R = arctan(k_{y,n'}^R/k_{x,n'}^R)$, n and n' are mode indexes, the reflection coefficient r_{mn} and transmission coefficient $t_{n'n}$ are to be determined. The y-component momentum is conserved, i.e., $\hbar k_n^L sin(\theta_n^L) = \hbar k_{n'}^R \times sin(\theta_{n'}^R)$ when Dirac fermions pass through the junction.

The continuity of the wave functions at $x = 0$ gives

$$\psi^L(x=0) = \psi^R(x=0), \quad (6)$$

and the current conservation of the systems at $x = 0$ gives

$$J_x^L \psi^L(x=0) = J_x^R \psi^R(x=0), \quad (7)$$

where

$$J_x^{L/R} = \begin{bmatrix} 2D_-k_x^{L/R} & 0 & 0 & A_2 \\ 0 & 2D_+k_x^{L/R} & A_2 & 0 \\ 0 & A_2 & 2D_-k_x^{L/R} & 0 \\ A_2 & 0 & 0 & 2D_+k_x^{L/R} \end{bmatrix} \quad (8)$$

is the current density matrix with $D_\pm = (D_2 \pm B_2)$. So the longitudinal wave vector $k_x^{L/R}$ and the eigenvector (with 4×1 blocks $\alpha_n^{L/R}$) are determined from the generalized eigenvalue problem

$$\begin{pmatrix} 0 & 1 \\ S & \zeta \end{pmatrix} \begin{pmatrix} \alpha \\ F \end{pmatrix} = k_x \begin{pmatrix} 1 & 0 \\ 0 & X \end{pmatrix} \begin{pmatrix} \alpha \\ F \end{pmatrix}, \quad (9)$$

where $F = k_x\alpha$. For the left region of the junction the matrices

$$S_{mn}^L = \begin{bmatrix} \Delta_{mn}^{L+} & -iA_1\eta_{mn} & 0 & 0 \\ -iA_1\eta_{mn} & \Delta_{mn}^{L-} & 0 & 0 \\ 0 & 0 & \Delta_{mn}^{L+} & iA_1\eta_{mn} \\ 0 & 0 & iA_1\eta_{mn} & \Delta_{mn}^{L-} \end{bmatrix}, \quad (10)$$

$$X_{mn}^L = \begin{bmatrix} -\xi_- & 0 & 0 & 0 \\ 0 & -\xi_+ & 0 & 0 \\ 0 & 0 & -\xi_- & 0 \\ 0 & 0 & 0 & -\xi_+ \end{bmatrix}, \quad (11)$$

$$\zeta_{mn}^L = \begin{bmatrix} 0 & 0 & 0 & A_2\Theta_- \\ 0 & 0 & A_2\Theta_- & 0 \\ 0 & A_2\Theta_+ & 0 & 0 \\ A_2\Theta_+ & 0 & 0 & 0 \end{bmatrix}, \quad (12)$$

where $\Delta_{mn}^{L\pm} = C - \epsilon \pm M + \langle\varphi_m(z) \mid V \mid \varphi_n(z)\rangle + (D_1 \mp B_1)\langle\varphi_m(z) \mid k_z^2 \mid \varphi_n(z)\rangle$ with electron energy ϵ, $\eta_{mn} = \langle\varphi_m(z) \mid k_z \mid \varphi_n(z)\rangle$, $\xi_\pm =$