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Surface States of Bi_2Se_3 Nanowires in the Presence of Perpendicular Magnetic Fields *

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We study the surface states of Bi_2Se_3 nanowires (NWs) in the presence of perpendicular magnetic fields. It is found that the minigap of Bi_2Se_3, arising from the quantized surface states around the circumference of NWs can be closed by perpendicular magnetic fields. With increasing magnetic fields, the Landau levels and edge states appear and localize at the center and edge of NWs, respectively. More interestingly, magnetic fields split the electron surface subbands with opposite tangential momenta, leading to specific edge states with low group velocity.

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Spin-orbit interaction (SOI) is a relativistic effect which could lead to many exotic physical phenomena. In conventional semiconductors with spacial inversion asymmetry, SOI is relatively weak and causes spin splitting and spin relaxation. In narrow bandgap materials consisting of heavy atoms, such as HgTe and Bi_2Se_3, SOI is strong so that it can lead to a band inversion between the conduction band and valence band. This results in a topological phase with an energy gap in the bulk and metallic surface or edge states at its boundary.[1−4] These materials with topological phases, named topological insulators (TIs), have attracted much attention of theorists and experimenters.[5−7] The predicted two-dimensional (2D) topological phase in HgTe quantum wells was shown to exhibit gapless helical edge states,[2,3,8,9] and the surface states in three-dimensional (3D) TIs, e.g., Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3,[10] were confirmed by angle-resolved photoemission spectroscopy.[11−14] These surface states can lead to novel magnetic properties.[15] Recently, TI has been proposed to be realized in commonly used semiconductors,[16,17] which suggests a promising approach to integrate TIs in well developed semiconductor electronic devices.

Semiconductor nanowires (NWs) are emerging as new nano-devices with an enormous potential for applications. The electronic states of a cylindrical two-dimensional electron gas (2DEG) in a transverse magnetic field were calculated by Ferrari *et al*,[18,19] and carbon nanotubes immersed in a perpendicular magnetic field were studied by Perfetto *et al.*[20,21] Novel single-crystal topological nanostructures can be grown by vapor-liquid-solid assisted by nanosize gold particles[22,23] or they can be realized by the so-called Scotch tape method.[24,25] TI NWs are an excellent system to investigate the properties of exotic surface states. Firstly, as the sample size shrinks, the contribution of surface states to electrical and optical properties is enhanced due to the increase of the surface-to-volume ratio. Secondly, compared to carbon nanotube, the radii of TI NWs can be large, so that magnetic fields weaker than 10 T can result in significant magnetic effects. While the effect of a magnetic field parallel to the TI NW axis is well known,[9,22,26−30] e.g., Aharonov–Bohm effect, the properties of TI NW surface states under a transverse magnetic field are less well understood. In this Letter, we investigate the effects of a transverse magnetic field on the electronic properties of Bi_2Se_3 NW surface states by looking at the possibility of the formation of Landau levels and edge states in such a closed geometry.

The Hamiltonian for surface states of the TI Bi_2Se_3 NW is given by the massless Dirac Hamiltonian on a curved surface, which can be simply expressed by[29,31,32]

$$\hat{H} = (\boldsymbol{n}_1\cdot\boldsymbol{\sigma}\cos\theta + \boldsymbol{n}_2\cdot\boldsymbol{\sigma}\sin\theta)(\boldsymbol{n}_1\cdot\boldsymbol{p}) + (\boldsymbol{n}_2\cdot\boldsymbol{\sigma}\cos\theta - \boldsymbol{n}_1\cdot\boldsymbol{\sigma}\sin\theta)(\boldsymbol{n}_2\cdot\boldsymbol{p}), \quad (1)$$

where θ is the angle between spin and momentum, and $\boldsymbol{n}_{1,2}$ are the orthogonal directions of the plane. For the surface states of the Bi_2Se_3 system, the electron spins are locked perpendicularly to their orbital momentum. Adopting cylindrical coordinate system (e_r, e_φ, e_z), the surface state Hamiltonian of the Bi_2Se_3 NW can be expressed simply by $H_{\rm surf} = v^{\rm F}\boldsymbol{n}_r\cdot(\boldsymbol{\sigma}\times\boldsymbol{p})_r = v^{\rm F}(\sigma_\varphi p_z - p_\varphi\sigma_z)$, where $\boldsymbol{n}_r$ is the unit vector perpendicular to the surface of the NW, and $v^{\rm F}$ is the Fermi velocity. The momentum operators are $p_z = -i\hbar\partial/\partial z$, and $p_\varphi =$

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$(\hbar/R)(-i\partial/\partial\varphi + \Theta)$, where the dimensionless flux parameter Θ comes from the effective magnetic field along the wire axis. It is interesting to notice that the Fermi velocities in the axial and tangent directions are anisotropic: in the axial direction, the Fermi velocity is $v_\varphi^{\rm F} = A_0\sqrt{1-(C_2/M_2)^2}\cdot {\rm nm}/\hbar \approx 0.6\times 10^6\,{\rm m/s}$, and in the tangent direction, the Fermi velocity is $v_z^{\rm F} = B_0\sqrt{1-(C_2/M_2)^2}\cdot {\rm nm}/\hbar \approx 0.3\times 10^6\,{\rm m/s}$. Taking this anisotropy into consideration, we rewrite the surface Hamiltonian as

$$H_{\rm surf} = \begin{pmatrix} -v_\varphi^{\rm F} p_\varphi & -iv_z^{\rm F} e^{-i\varphi} p_z \\ iv_z^{\rm F} e^{i\varphi} p_z & v_\varphi^{\rm F} p_\varphi \end{pmatrix}. \quad (2)$$

When there is no magnetic field (or if there is a magnetic field along the NW axis), the total angular momentum is a good quantum number, $[H, L_z + S_z] = 0$. The surface states satisfy the Schrödinger equation $H_{\rm surf}\psi^{\rm s} = E\psi^{\rm s}$, in which the surface state wave function $\psi^{\rm s}$ can be written as

$$\psi^{\rm s} = \chi e^{ij\varphi} e^{ik_z z}, \quad (3)$$

where $j = \ldots, -\frac{3}{2}+\Theta, -\frac{1}{2}+\Theta, \frac{1}{2}+\Theta, \frac{3}{2}+\Theta, \ldots$, and $\chi = (e^{-i\frac{\varphi}{2}}\xi_1, e^{i\frac{\varphi}{2}}\xi_2)^T$. The secular equation becomes

$$\begin{pmatrix} \frac{-v_\varphi^{\rm F}}{R}\left(j-\frac{1}{2}\right)\hbar & -iv_z^{\rm F}\hbar k_z \\ iv_z^{\rm F}\hbar k_z & \frac{v_\varphi^{\rm F}}{R}\left(j+\frac{1}{2}\right) \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = E \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}. \quad (4)$$

The energy dispersion can be obtained analytically as follows:

$$E_\pm = \frac{v_\varphi^{\rm F}\hbar}{2R} \pm \hbar\sqrt{(v_z^{\rm F})^2 k_z^2 + \frac{j^2(v_\varphi^{\rm F})^2}{R^2}}, \quad (5)$$

where the sign $\pm$ refers to the conduction and valence bands, respectively. Due to the spatial reversal symmetry, the states $|k_z, j\rangle$ and $|-k_z, j\rangle$ are degenerate. Here χ can be expressed by

$$\chi_+ = \begin{pmatrix} [h(j)\sin\frac{\theta}{2} + h(-j)\cos\frac{\theta}{2}]e^{-i\frac{\varphi}{2}} \\ [h(j)\cos\frac{\theta}{2}e^{i\gamma} + h(-j)\sin\frac{\theta}{2}e^{i\gamma}]e^{i\frac{\varphi}{2}} \end{pmatrix}, \quad (6a)$$

$$\chi_- = \begin{pmatrix} [h(j)\cos\frac{\theta}{2} + h(-j)\sin\frac{\theta}{2}]e^{-i\frac{\varphi}{2}} \\ [-h(j)\sin\frac{\theta}{2}e^{i\gamma} - h(-j)\cos\frac{\theta}{2}e^{i\gamma}]e^{i\frac{\varphi}{2}} \end{pmatrix}, \quad (6b)$$

where $h(x)$ is the Heaviside step function, $\gamma = \frac{\pi}{2}$ (when $k_z \geq 0$) or $-\frac{\pi}{2}$ (when $k_z < 0$), and $\tan\theta = |v_z^{\rm F} k_z/[jv_\varphi^{\rm F}/R]|$. Note that the effective angular momentum j includes the contribution from the effective magnetic field along the NW axis. There is a mini gap $(v_\varphi^{\rm F}\hbar/R)$ at $k_z = 0$, which arises from the quantize surface states around the circumference of the NW. Therefore, from the mini gap and the Fermi velocity along the φ direction, we can obtain the size of the NW. The mini gap can be closed by applying a magnetic field (i.e., $j + \Theta = 0$) along the NW axis.

Suppose that the NW is along the z-direction. We now consider a magnetic field perpendicular to the NW axis (as shown in Fig. 1(a)), which is supposed to be along the y direction $\boldsymbol{B} = [0, B, 0]$. The vector potential is $\boldsymbol{A} = [0, 0, -xB]$. In the cylindrical coordinate system, the vector potential is $\boldsymbol{A} = [0, 0, -r\cos\varphi B]$. When the magnetic field is perpendicular to the axis of the wire, the total angular momentum project on the z axis is no longer a good quantum number. In this cylindrical coordinate system, we rewrite the wave vector operator as $\hat{k}_\rho = -i\partial/\partial\rho$, $\hat{k}_\varphi = (-i/\rho)\partial/\partial\varphi$, $\hat{k}_z = -i\partial/\partial z - er\cos\varphi B(z)/\hbar$.

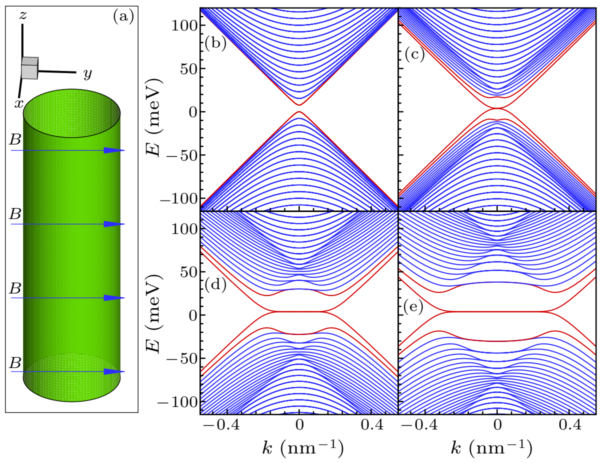

Fig. 1. (Color online) (a) Sketch of the NW. The magnetic field $\boldsymbol{B}$ (blue line) is along the y direction. Here (b), (c), (d) and (e) are the energy spectra of Bi_2Se_3 NW with $R = 50\,{\rm nm}$ in different magnetic field $B = 0\,{\rm T}$, $B = 1\,{\rm T}$, $B = 3\,{\rm T}$ and $B = 5\,{\rm T}$, respectively.

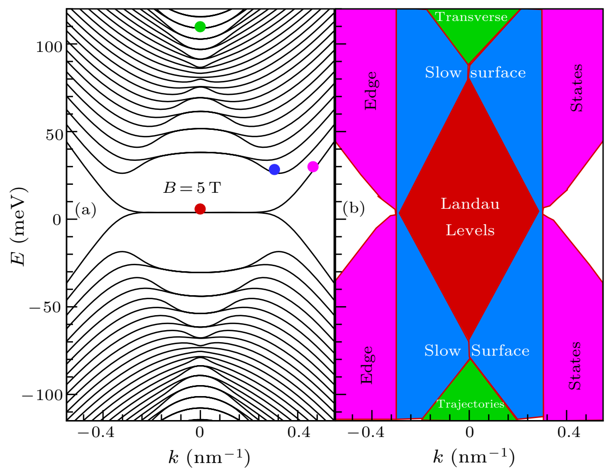

Fig. 2. (Color online) (a) The energy spectrum of Bi_2Se_3 NW with $R = 50\,{\rm nm}$ with magnetic field $B = 5\,{\rm T}$. (b) The phase diagram corresponding to (a).

We consider a cylinder immersed in a homogeneous magnetic field $\boldsymbol{B}$. The system has translation invariance along the z direction. We can expand the wave function by a plane wave in z direction

$$\psi = e^{ik_z\cdot z}\sum_m \begin{pmatrix} a_m\frac{1}{\sqrt{2\pi}}e^{im\varphi} \\ b_m\frac{1}{\sqrt{2\pi}}e^{im\varphi} \end{pmatrix}. \quad (7)$$

We can obtain the Hamiltonian matrix element by the formula: $\int_0^{2\pi}[\hbar k_z - eBr\cos(\varphi)]e^{iN\varphi}d\varphi = \hbar k_z\delta_{N,0} - eBr(\delta_{N+1,0}+\delta_{N-1,0})/2$. From this formula, we can see that the external magnetic field coupling the state $|m\rangle$ with $|m\pm 1\rangle$ state and the $L_z + S_z$ is no longer a good quantum number. We should solve the Schrödinger equation $H_{\rm surf}\psi^{\rm s} = E\psi^{\rm s}$ numerically. Figures 1(b), 1(c), 1(d) and 1(e) show the energy spectrum of Bi_2Se_3 NW surface states in perpendicular magnetic fields. Without the magnetic field (as shown in Fig. 1(b)), all states are doubly degenerate which is required by the time reversal symmetry. The red lines denote the conduction band minimum (CBM) and valence band maximum (VBM), correspondingly the angular momentum $j = \pm\frac{1}{2}$. In Fig. 1(b), there is a mini gap, which is arising from the quantized surface states around the circumference of NW. It has been reported that this mini gap can be closed by magnetic fields parallel to the TI NW axis.[9,22,26−29] We find that, with the increasing strength of the perpendicular magnetic fields, the mini gap of the Bi_2Se_3 NW can also be closed (as shown in Figs. 1(c), 1(d), and 1(e)). The two-fold degeneracy is lifted by the magnetic fields for the low energy levels at finite wave vector. It is interesting that a flat band region, quasi-Landau levels, can be realized by the surface states on the cylinder surface (as shown in Figs. 1(c), 1(d), 1(e)). The presence of the gapless lowest Landau level in strong magnetic field is a typical character of Dirac fermions.

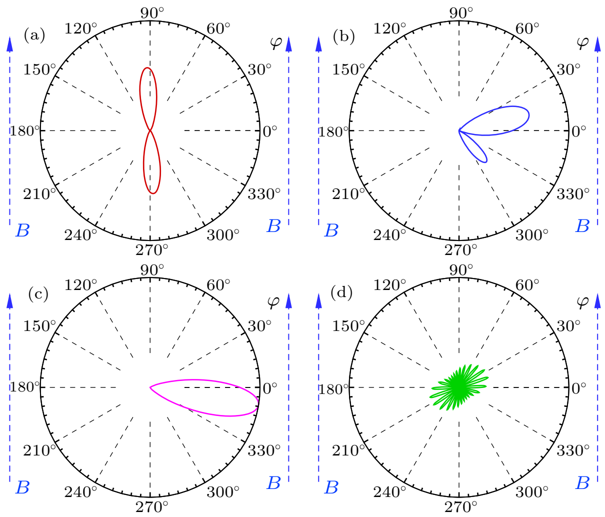

Fig. 3. (Color online) (a), (b), (c) and (d) are the wave function distribution of Landau level region, slow edges region, edge states region and transverse trajectory region, respectively. The chosen states are denoted in Fig. 2(a) as red, blue, pink and green points, respectively. The blue dashed lines denote the direction of magnetic field.

To see the effects of magnetic fields on the surface states of NWs more clearly, we show the phase diagram in Fig. 2. When the magnetic fields are large enough, the energy-momentum space is divided into four regions. These four regions are named as quasi-Landau levels, slow surface, edge states and transverse trajectories regions, which are denoted as red, blue, pink and green regions, respectively (as shown in Fig. 2(b)).

Firstly, for strong magnetic fields the lowest subbands show pronounced flat edge regions near $k_z = 0$, corresponding to Landau levels (red region in Fig. 2(b)). By increasing magnetic fields $\boldsymbol{B}$, the energy becomes almost independent of the wave vector in a large range and approaches the value of Landau levels in a planar 2D system. Moreover, notice that the level spacing between adjacent Landau levels is not equally spaced since $\varepsilon_n \propto \sqrt{n}$ as is typical for relativistic Dirac particles. The electrons are located at the top (bottom) of the NWs, which can be seen in Fig. 3(a).

Secondly, in the slow surface region (blue region in Fig. 2(b)), the energy first decreases with wave vector and then increases with wave vector. The energy levels have the minimum energy in this region. This minimum energy can be understood by the shift minimum of two parabolas. Since

$$\begin{pmatrix} -v_\varphi^{\rm F}p_\varphi & -iv_z^{\rm F}e^{-i\varphi}p_z \\ iv_z^{\rm F}e^{i\varphi}p_z & v_\varphi^{\rm F}p_\varphi \end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = E\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}, \quad (8)$$

we can obtain

$$E = \pm\sqrt{(v_\varphi^{\rm F}p_\varphi)^2 + (v_z^{\rm F}p_z)^2}, \quad (9)$$

where $p_z = \hbar k_z - eBR\cos(\varphi)$. When $\cos(\varphi) > 0$ ($\cos(\varphi) < 0$), the minimum of one parabola's shift to the right (left). From Eq. (9), when the momentum k_z is not very large, electrons with opposite tangential momenta $|\pm m\rangle$ will be split, since the magnetic field couples the $|m\rangle$ and $|m\pm 1\rangle$, the angular momentum $|m\rangle$ is no longer a good quantum number. The coupling splits the surface subbands. With the increasing momentum k_z, the lower branch energy increases at large momentum k_z (see Eq. (9)). Therefore one can see that the surface Landau levels shift to one side, while still not approaching the edges. These states possess low group velocities. We call it slow surface states. The electrons are located at the left (or right) sides of the NW, which can be seen in Fig. 3(b).

Thirdly, in the edge states region (pink region in Fig. 2(b)), electrons are located on the left flank (or right flank) according to whether they have a positive (or negative) velocity (i.e., momentum k_z), which is shown in Fig. 3(c).

Fourthly, in transverse trajectories region (green region in Fig. 2(b)), electrons are almost located at the cross section of NWs, therefore we call this region the transverse trajectory region as shown in Fig. 3(d).

In summary, we have investigated theoretically the surface states of TI Bi_2Se_3 NWs in the presence of perpendicular magnetic fields. We find that the mini gap of the Bi_2Se_3 NWs, arising from the quantized surface states around the circumference of NW, can be closed by perpendicular magnetic fields. When the magnetic fields are large enough, the energy-momentum space is divided into four regions. Quasi-Landau levels can be realized by the surface states on the cylinder surface. The level spacing between adjacent Landau levels is not equally spaced as is typical for relativistic Dirac particles. Electrons in the edge state region are located at the flank of NW and electrons in transverse trajectory region are located at the cross section of NW. Our theoretical result is interesting from both the basic physics and potential application of the spintronic devices based on this Bi_2Se_3 nanowire.

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