Quantum Hall effect of the surface states in topological insulator

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We study the quantum Hall effect in the surface states of topological insulator in the presence of a perpendicular magnetic field in the framework of edge states. Motion of Dirac fermions will form discrete Landau levels, among which a fully saturated zero mode will have different behaviors near the boundary according to the sign of the effective mass for Dirac fermions. The Hall conductance is quantized to be $ne^2/h$ ($n$ is an integer) for a positive mass, $(n + 1)e^2/h$ for a negative mass, and $(n + 1/2)e^2/h$ for massless fermions. In topological insulator the massive term $m_{\text{eff}}$ to the Dirac fermions can be the Zeeman coupling in a magnetic field or be induced by the finite-size effect in an ultrathin film. For example the g-factor of Bi$_2$Se$_3$ is positive and give rise to a positive mass term for Dirac fermions. We address experimental realization of the quantum Hall effect in topological insulators.

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Three-dimensional topological insulators possess metallic surface states in a band gap which reside near the system surface as a consequence of strong spin-orbit coupling.

Recent experiments and the first principles calculations have verified the existence of this novel type of topological states in the materials such as Bi$_{1-x}$Se$_x$, Bi$_2$Se$_3$, and Bi$_2$Te$_3$. The surface states have linear dispersion in the momenta and are modeled as a two-dimensional free Dirac fermion gas, which is analogous to a single layer graphene. The Hall conductance of two-dimensional Dirac fermions is well defined only when the mass $m_{\text{eff}}$ of the fermions is nonvanishing, $\sigma_H = \text{sgn}(m_{\text{eff}}) \frac{e^2}{\hbar}$. In the presence of a perpendicular and uniform magnetic field, it was predicted that the Hall conductance of massless Dirac fermions is quantized as $n e^2/h$ (n is an integer). The charge carriers in a single layer graphene are regarded as massless Dirac fermions, and the measured quantum Hall conductance is $4(n + 1/2)e^2/h$ where the factor 4 originates from the spin and valley degeneracy. However, strictly speaking, the measured quantity in graphene is $2e^2/h$, not $e^2/2h$ directly. The newly discovered topological insulator Bi$_2$Se$_3$ and Bi$_2$Te$_3$ have been identified to have a single Dirac cone which may provide an ideal platform to study a half of the quanta $e^2/h$ for the Hall conductance. On the other hand, the conventional edge state picture for quantum Hall effect have established an explicit relation between the Chern number or the quantized Hall conductance and the number of the edge states. A half-quantized Hall conductance are challenging the validity or applicability of the edge state theory if the quantum Hall effect exist in the surface states of topological insulators.

In this paper we study the quantum Hall effect for a two-dimensional Dirac fermions in the presence of a magnetic field in the edge state theory. The Landau level formation will lead to the quantization of the quantum Hall conductance. It is found that a fully saturated zero mode of the Landau level appears, and its edge effect near the boundary determines its contribution to the quantum Hall conductance. The sign of the effective mass of Dirac fermions plays a decisive role. For Dirac fermions of positive mass, the Hall conductance is $ne^2/h$ as a conventional two-dimensional electron gas, for Dirac fermions of negative mass, the Hall conductance is $(n + 1)e^2/h$, and for massless Dirac fermions the Hall conductance is $(n + 1/2)e^2/h$. These results can be applied to the surface states of topological insulator and an ultra-thin film of topological insulator. Since the surface states in topological insulator has a spin texture structure, which is distinct from the Dirac cone in graphene, the application of magnetic field breaks the time reversal symmetry and the Dirac fermions in the surface states acquire a massive term, i.e., the Zeeman term. Thus the sign of the g-factor will determined the value of quantum Hall conductance. For example the g-factor in Bi$_2$Te$_3$ is positive and generates a positive mass. As a result the quantum Hall conductance is $ne^2/h$, which is identical as a conventional two-dimensional electron gas. For an ultra-thin film, the finite size confinement will mix the surface states at the top and bottom layers and generate an energy gap for Dirac fermions. Since the system is still invariant under time reversal symmetry, one set of fermions possesses positive mass and another set possesses negative mass. As a result the Hall conductance can be $2(n + 1/2)e^2/h$ if the energy gap is larger than the Zeeman splitting.

We start with a 2+1 massive Dirac Hamiltonian

$$H = v_F h(k_x \sigma_x + k_y \sigma_y) + m_{\text{eff}} v_F^2 \sigma_z$$

where $v_{\text{eff}}$ is the effective speed of light and $m_{\text{eff}}$ is the effective mass. $\sigma_{x,y,z}$ are the Pauli matrices. To calculate the Hall conductance the Hamiltonian can be written in the form, $H = d(k) \cdot \sigma$ with the vector $d(k) = (v_F h k_x, v_F h k_y, m_{\text{eff}} v_F^2)$. The Hall conductance of the Dirac fermions is only well defined in a massive case,

$$\sigma_H = \frac{e^2}{2\hbar} \sum_k \frac{\text{sgn}(m_{\text{eff}}) e^2}{|d(k)|^3} = \text{sgn}(m_{\text{eff}}) \frac{e^2}{2\hbar}$$
when the Fermi energy is located between the band gap. For a non-interacting system, it is impossible to have a half-quantized Hall conductance in unit of $e^2/h$. However, the sign change of the mass $m_{eff}$ will lead to a jump of Hall conductance, i.e., $\Delta \sigma_H = \frac{\pi}{2}$.

Now we come to study the formation of the Landau levels with a finite boundary following the theories of edge states by Halperin and MacDonald and Stradling. We first consider a geometry of strip with a width $L_y$ and thickness $H$, which are much larger than the magnetic length $l_B$ and the spatial distribution $\xi$ of the surface states. Assume the magnetic field $B$ (alone the z-axis) is perpendicular to the slab as shown in Fig. 1(a). We first focus on the top plane. The periodic boundary condition is taken along the x-axis, and the open boundary condition along the y-axis. In this way the number $k_x$ is still a good quantum number, and $k_y$ is substituted by $-i\partial_y$. We take the Landau gauge for the vector potential, $A_x = +By$ and $A_y = 0$. Thus we define $a(y_0) = \frac{L_y}{\sqrt{2}}[\partial_y + l_B^{-2}(y-y_0)]$ where the magnetic length $l_B = \sqrt{\hbar/eB}$ and $y_0 = -l_B^2k_x$ assuming $eB > 0$.

The operators $a$ and $a^\dagger$ satisfy the commutation relation, $[a(y_0), a^\dagger(y_0)] = 1$. For simplicity, we introduce a dimensionless parameter $\delta = m_{eff}v_F^2l_B/\sqrt{2}\hbar v_F$. In this way, we have a dimensionless Schrodinger equation,

$$\begin{pmatrix} \delta & a \\ a^\dagger & -\delta \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} = \frac{E}{v_F\sqrt{2\hbar eB}} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}.$$  

The allowed values for $y_0$ are separated by $\delta y_0 = 2\pi l_B^2/L_y$ with a periodic boundary condition with length $L_y$ and are limited within $0 < y_0 < L_y$. The solution is a function of the good quantum number $k_x$ or $y_0 = -l_B^2k_x$. When $y_0$ is far away from two edges of $y = 0$ and $y = L$, the two components $\varphi_1$ and $\varphi_2$ will vanish at the two boundaries. In this case, the energy eigenstates are

$$|n, \alpha\rangle = \left(\begin{array}{c} \sin \theta_{n,\alpha} |n-1\rangle \\ \cos \theta_{n,\alpha} |n\rangle \end{array}\right)$$

where $\tan \theta_{n,\alpha} = \frac{\sqrt{n}}{\alpha\sqrt{n+\delta^2}}$, $\alpha = \pm 1$, $n$ is a positive integer, $|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger(y_0))^n|0\rangle$ the solution for a simple harmonic oscillator and $a(y_0)|0\rangle = 0$. The Landau energy is given by

$$E_{n,\alpha} = \alpha v_F \sqrt{2\hbar B (n + \delta^2)}$$

for a positive integer $n$, which are highly degenerate.

It should be emphasized that the zero mode $E_0 = -v_F\sqrt{2\hbar B\delta}$ for $n = 0$ and the eigenstate is totally saturated, $|0, 0\rangle = \left(\begin{array}{c} 0 \\ 1 \end{array}\right)$. The number of the allowed values of $y_0$, $N_L/L_y/\delta y_0 = 2\pi L_x L_y/l_B^2$, is the degeneracy of the Landau levels. The energy expressions yield an energy gap $\Delta E = |E_{n=\pm 1}| - E_0$ between the zero mode and the states of $n = \pm 1$. For $\delta = 0$ the energy gap is about $\Delta E \approx 800$K for Bi$_2$Se$_3$ at $B = 10$T, which makes it possible that the quantum Hall effect can be measured even at room temperature just as in single layer graphene.

The boundary effect will remove the degeneracy of the Landau level when $y_0$ is near the boundary. It was known that we cannot simply take a rigid wall condition such that the two components $\varphi_1$ and $\varphi_2$ vanish simultaneously at the boundary. No solution in Eq. (3) will satisfy this type of boundary conditions. In the graphene it is a common practice to calculate the boundary effect numerically in the tight binding approximation. In the present case, since the surface state has a finite spatial distribution, we do not expect the two components $\varphi_1$ and $\varphi_2$ will vanish simultaneously near the boundary. We first focus on the boundary effect to the zero mode. After some algebra, we have a expression for the zero energy mode

$$E_{y_0} = -\text{sgn}(\delta)v_F\sqrt{2\hbar B(v_0 + \delta^2)}$$

where $\nu_0 = \langle\varphi_2|a^\dagger(y_0)a(y_0)|\varphi_2\rangle/\langle\varphi_2|\varphi_2\rangle$. The sign of $\delta$ guarantees the continuity of the spectrum from the bulk to the edge. When $0 < y_0 < L_y$, $\nu_0 = 0$ and $\varphi_2(y, y_0) \propto |y/n = 0\rangle = \frac{1}{\pi^{1/4}l_B^{1/2}} \exp[-(y-y_0)^2/2l_B^2]$. If the boundary condition makes $\varphi_2 = 0$ for $y_0 = 0$ we have a solution for $\varphi_2(y, y_0 = 0) \propto |y/n = 1\rangle = \frac{1}{\pi^{1/4}l_B^{1/2}} y \exp[-y^2/2l_B^2]$. In this case $\nu_0 = 1$, but in this case $\varphi_1(y, y_0) \propto |y/n = 0\rangle$. The value of $\nu_0$ varies from 0 to 1 when $y_0$ moves from the bulk to $y_0 = 0$ or $L_y$. In another limit, if we take $\varphi_1 = 0$ for $y_0 = 0$, the solution $|0, 0\rangle = \left(\begin{array}{c} 0 \\ 1 \end{array}\right)$ and is not distorted by the boundary at all, which is apparently unphysical. It will be reasonable to assume $0 < \nu_0 < 1$ near the boundaries.
which is between these two limits, since the boundaries should distort the Gaussian-type wave function in the bulk \((0 << y_0 << L_0)\). For a negative \(\delta\), the spectra of the Landau levels goes upward near the boundary because fermions of positive mass, but for a positive \(\delta\) the spectrum goes like fermions of negative mass. For massless fermions of \(\delta = 0\), the energy spectra near the boundary have two possible solutions, \(E_{\nu_0} = +v_F \sqrt{2e\hbar B\nu_0}\) and \(E_{\nu_0} = -v_F \sqrt{2e\hbar B\nu_0}\). Consider the particle-hole symmetry. We may say half of the particles in the zero mode have positive energy while another half of the particles have negative energy. For other states of an integer \(n\), \(\nu_n = \langle \varphi_2 \rvert a^\dagger(y_0) a(y_0) \rvert \varphi_2 \rangle / \langle \varphi_2 \rvert \varphi_2 \rangle\) is between \(n\) (in the bulk) and \(2n + 1\) near the edge boundary. In general case, we plot the energy spectra schematically in Fig. 1(b), (c) and (d) according to the value of \(\delta\).

According to the sign of the mass, \(m_{\text{eff}}\), these energy spectra near the boundary will lead to three different results for quantum Hall conductance. For \(\delta < 0\), the zero mode has the same behaviors of the states of \(n > 0\) and \(\alpha = +1\): the spectrum goes upward near the boundary. It will generate an edge current. Following MacDonald and Streda, the edge current is given by

\[
I_{n=0} = \frac{1}{\delta y_0} \int_0^{L_y} dy_0 \frac{e^2}{h} \frac{\hbar}{\mu} \frac{\partial E_{\nu_0}(y_0)}{\partial y_0} \Theta(\mu - E_{\nu_0}(y_0))
= \frac{e}{h} (\mu^R - \mu^L),
\]

where \(\mu^R, L\) are the potentials at the two sides. This will contribute one \(e^2/h\) to the Hall conductance. Thus the Hall conductance should be \(\sigma_{xy} = (n + 1) \frac{e^2}{h}\) for \(\delta < 0\) when other \(n\) Landau levels above the zero mode are filled. For \(\delta > 0\), the energy spectrum goes downward near the boundary. The zero mode will not contribute to the Hall conductance when the Fermi energy is above the zero mode, \(E_f > E_{\nu_0}\), and thus the Hall conductance is \(n \frac{e^2}{h}\), which is the quantum Hall conductance for a conventional two-dimensional electron gas. The massless case of \(\delta = 0\) is special since the spectra near the boundary can go either upward or down-ward. We may say half of the fermions in the zero modes have positive mass, and another half have negative mass. In this case the zero mode will contribute one half of the quantum \(\frac{e^2}{h}\) to the Hall conductance. As a result, the Hall conductance should be \((n + \frac{1}{2}) \frac{e^2}{h}\), which is in agreement with the previous results. In short, the quantum Hall conductance for the surface states is determined by the sign of \(\delta\) or \(m_{\text{eff}}\),

\[
\sigma_H = \begin{cases} 
(n + 1) \frac{e^2}{h} & \text{if } \delta < 0 \\
(n + \frac{1}{2}) \frac{e^2}{h} & \text{if } \delta = 0 \\
n \frac{e^2}{h} & \text{if } \delta > 0 
\end{cases}
\]

Now turn to apply these results to the Dirac fermions in the surface states of topological insulators. The Dirac fermions are massless and the Dirac point is protected by the time reversal symmetry, and is robust against impurities or defects. Since the Dirac fermions carries real spin with a texture structure in the momentum space, a Zeeman splitting will be induced when the system is subjected to a perpendicular magnetic field, \(g_{\text{eff}} \mu_B \sigma_z\), which is equivalent to the effective mass term \(m_{\text{eff}} = g_{\text{eff}} \mu_B / v_F^2\). Thus the sign of the \(g\)-factor will determine the value of quantum Hall conductance as in Eq. (\ref{eq:8}). For example in Bi\(_2\)Se\(_3\), numerical estimation of the value \(g_{\text{eff}}\) from the tight binding approximation is about \(g_{\text{eff}} = 1.8\). This illustrates that the Dirac fermions in the surface states acquires a positive mass in the presence of a perpendicular magnetic field. From this result, we conclude that the quantum Hall conductance of the surface states in Bi\(_2\)Se\(_3\) is \(\frac{e^2}{h}\) as in two-dimensional electron gas.

Consider the magnetic field normal to the top and bottom surfaces of a sample as shown in Fig. 1. The surface states of all lateral sides just experience a in-plane field, in which the main effect of magnetic field is the Zeeman coupling. We have discussed the quantum Hall conductance in the top surface. If we assume the magnetic field \(B\) is along the z-direction, normal to the top surface, the electrons in the bottom surface will equivalently experience a \(-B\) field. In this case, the operators \(a\) and \(a^\dagger\) in the effective model (Eq. (\ref{eq:3})) for the bottom surface fermions should be re-defined: \(a\) operator should be replaced by \(a^\dagger\) and vice versa. The \(\delta\)-term is attributed to the Zeeman term, it will also change its sign, \(\delta \rightarrow -\delta\). As a result, the zero energy mode will change to \(|0, 0\rangle = \begin{pmatrix} |0\rangle \\ 0 \end{pmatrix}\) and the energy remains unchanged, \(E_0 = -v_F \sqrt{2e\hbar B}\). Thus we conclude that the Hall conductance \(\sigma_{xy}\) of the bottom surface is identical to the top surface, and there is no voltage drop between the top and bottom surface states. Thus the total Hall conductance should be \(2ne^2/h\) \((g_{\text{eff}} > 0)\) or \(2(n + 1)e^2/h\) \((g_{\text{eff}} < 0)\). These properties will make feasible to measure the quantum Hall effect of the topological surface states.

The finite size effect of the surface states will generate different quantum Hall effect in an ultra-thin film of topological insulator. When the spatial distribution of the wave function of the surface states is comparable with the thickness of the thin film, the quantum tunneling of the wave functions of the top and bottom surface states will generate an energy gap in the dispersion of Dirac fermions. Since the system is still invariant under the time reversal symmetry, the two sets of Dirac fermions, as a mixture of the top and bottom surface states, will acquire positive and negative masses, \(m_{\text{eff}} = \tau \frac{e^2}{h}\) with \(\tau = \pm 1\), respectively. The energy gap is estimated to be about 0.13eV when the thickness of thin film is 20Å. The effective mass term for Dirac fermions in an ultra-thin film becomes

\[
\Delta H = (\tau \frac{e^2}{h} + g_{\text{eff}} \mu_B B) \sigma_z.
\]
will be determined by the sign of the g-factor. However, if the gap is larger than the Zeeman splitting, the effective mass is positive for one set of fermions and negative for another set. In this case the quantum Hall conductance for the two sets of Dirac fermions are \((n + 1 \frac{e^2}{h})\) and \(n \frac{e^2}{h}\), respectively. As a result the total quantum Hall conductance is \(2(n + \frac{1}{2}) \frac{e^2}{h}\), which looks like the Hall conductance for doubly degenerated and massless Dirac fermions. Lee et al. obtained the quantized Hall conductance \(2(n + \frac{1}{2}) \frac{e^2}{h}\) in the same geometry, which is consistent with the present result by neglecting the Zeeman splitting.

In conclusion, the Zeeman coupling will be induced as a mass term for Dirac fermions in the topological surface states in the presence of a magnetic field. From the point of view of edge states, the sign of the effective g-factor or mass determines the dispersion behaviors of Landau levels near the boundary, and further the value of the quantum Hall conductance of the Dirac fermions. For \(\text{Bi}_2\text{Se}_3\) the calculated g-factor is positive, or equivalently the Dirac fermions have positive mass, which gives rise to the quantum Hall conductance \(2ne^2/h\) as the conventional two-dimensional electron gas. For an ultra-thin film, the finite-size effect will open an energy gap for Dirac fermions. If the gap is smaller than the Zeeman splitting, the Hall conductance is \(2ne^2/h\) while if it is larger than Zeeman splitting, the quantum Hall conductance is \(2(n + \frac{1}{2}) \frac{e^2}{h}\).

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