Quantized Conductance and Field-Effect Topological Quantum Transistor in Silicene Nanoribbons

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Silicene (a monolayer of silicon atoms) is a quantum spin-Hall insulator, which undergoes a topological phase transition into other insulators by applying external field such as electric field, photo-irradiation and antiferromagnetic order. We investigate the electronic and transport properties of silicene nanoribbons based on the Landauer formalism. We propose to determine topological phase transitions by measuring the density of states and conductance. The conductance is quantized and changes its value when the system transforms into different phases. We show that a silicene nanoribbon near the zero energy acts as a field-effect transistor. This transistor is robust though it makes use of the minimum quantized conductance since the zero-energy edge states are topologically protected. Our findings offer a new way to future topological quantum devices.

Silicene is a honeycomb structure of silicon atoms akin to graphene. Its experimental synthesis has opened a breakthrough in the study of silicene. It has two salient features absent in graphene. One is the relatively large spin-orbit (SO) interaction, which enables quantum spin-Hall (QSH) effects to realize. The other is its buckled structure, which enable us to apply different external fields between the A and B sublattices such as electric field and exchange field. As a result we can externally tune the band gap of silicene and drive topological phase transitions from the QSH insulator to other insulators. We have already shown how to make experimental observation of phase transition points with the use of diamagnetism and also optical absorption. However, these methods may not be so practical.

The most important graphene derivative is nanoribbon. The low-bias low-temperature conductance \( \sigma \) of graphene nanoribbons has been shown to be quantized as

\[
\sigma = 4 (n + 1/2) (e^2/h), \quad n = 0, 1, 2, \ldots
\]

both for zigzag and armchair edges. We interpret the formula to imply the electron-hole symmetry, the 4-fold degeneracy of each energy level associated with the spin and valley degrees of freedom, and the conductance quantum \( e^2/h \) per channel. It is interesting to examine the same problem in silicene nanoribbons because the spin-valley degeneracy is broken according to a specific pattern in each phase.

Topological insulators are indexed by a set of two topological numbers \((C, C_s)\), where \(C\) and \(C_s\) are the Chern number and the spin-Chern number modulo 2. There appear four types of insulators in silicene. They are the QSH, the quantum anomalous Hall (QAH), the spin-polarized quantum anomalous Hall (SQAH), and the trivial band insulators. The QSH effect is an analogue of the quantum Hall effect for spin currents instead of charge currents. The QAH effect is the quantum Hall effect without Landau levels, while the SQAH insulator has a hybrid character of the QSH and QAH insulators. The prominent feature of a topological insulator is the emergence of zero-energy edge states at half-filling which are topologically protected against perturbation.

In this paper we calculate the density of states (DOS) and the conductance in zigzag silicene nanoribbons based on the Landauer formalism, and propose an experimentally better method to detect a topological phase transition by way of measuring them. Our first observation is that there are finite DOS due to the zero-energy edge states in a topological phase, while they are absent in the trivial phase. Consequently, the topological phase transition must be observed experimentally just by measuring the site-resolved DOS with controlled electric field, which can be achieved by spatially resolved the scanning tunneling microscopy/STM/STS.

The particularly important quantity is the conductance due to the topologically protected zero-energy edge channels, which is the one experimentally observable. It is interesting that the helical edge of the QSH and the chiral edge of the QAH insulators have the same amount of conductance. Our result is summarized as

| topological insulator | QAH | QSH | SQAH | trivial |
|----------------------|-----|-----|------|--------|
| topological numbers  | (2,0)| (0,1)| (1,1/2)| (0,0)  |
| conductance (\(\sigma\)) | 2   | 2   | 1    | 0      |

The conductance changes its quantized value when the system is transformed into different phases by tuning electric field. Because of this property a silicene nanoribbon may act as a field-effect transistor, where the conductance is quantized and topologically protected.

Hamiltonian: The basic nature of silicene is described by the tight-binding Hamiltonian

\[
H = -t \sum_{\langle i,j \rangle} c_{i\alpha}^\dagger c_{j\alpha} + i \frac{\lambda_{SO}}{3\sqrt{3}} \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} c_{i\alpha}^\dagger \sigma_2^{\alpha\beta} c_{j\beta},
\]

where \(c_{i\alpha}^\dagger\) creates an electron with spin polarization \(\alpha\) at site \(i\) in a honeycomb lattice, and \(\langle i, j \rangle / \langle\langle i, j \rangle\rangle\) run over all the nearest/next-nearest-neighbor hopping sites. The first term represents the usual nearest-neighbor hopping with the transfer energy \(t = 1.6 eV\). The second term represents the effective SO interaction with \(\lambda_{SO} = 3.9 m eV\), and \(\nu_{ij} = +1\) if the next-nearest-neighbor hopping is anticlockwise and \(\nu_{ij} = -1\) if it is clockwise with respect to the positive \(z\) axis. We have neglected the Rashba interactions since their effects are negligibly small in general. Here, \(\sigma_2\) is the Pauli matrix for the \(z\) component of the spin, whose eigenvalues are \(s_z = \pm 1\). We also use \(s_z = \uparrow \downarrow\) for indices.
Introducing photo-irradiation $\lambda$, the potential term $M$ where $v$ nothing but the SO coupling term with $\lambda$. The Hamiltonian is given by the massive Dirac theory around the $K$ point. The Hamiltonian yields

$$H_\eta^0 = \hbar v_F (\eta k_x \tau_x + \eta k_y \tau_y) + \lambda_{SO} \eta \tau_z \sigma_z, \quad (4)$$

where $v_F = \frac{\sqrt{3}}{2}a$ is the Fermi velocity with the lattice constant $a = 3.86\text{Å}$. Here, $\tau_z$ is the Pauli matrix for the $z$ component of the pseudospin representing the $A$ and $B$ sublattices, whose eigenvalues are $\tau_z = \pm 1$.

A great merit of silicene is that we can introduce various potential terms into the Hamiltonian by making advantages of its buckled structure. Eight commuting terms are possible in the Dirac Hamiltonian [4].

$$H_{pq} = \lambda_{pq} \eta^p (\sigma_z)^q (\tau_z)^r, \quad (5)$$

where $p, q, r = 0$ or $1$. Each term has different symmetry properties. The coefficient of $\tau_z$ is the Dirac mass, to which four terms contribute. They are $H_{pq1}$. First, $H_{111}$ is nothing but the SO coupling term with $\lambda_{111} = \lambda_{SO}$. Second, $H_{001}$ is the staggered sublattice potential term with $\lambda_{001} = \ell E_z$, where $\ell$ is the separation between the $A$ and $B$ sublattices and $E_z$ is the external electric field. Third, $H_{101}$ is the Haldane term [3], where we set $\lambda_{101} = \lambda_\Omega$ by introducing photo-irradiation $\lambda$. Finally, $H_{011}$ is the the staggered exchange term [5], where we set $\lambda_{011} = \Delta M = M_A - M_B$ by introducing the exchange fields $M_{A,B}$ to the $A(B)$-sublattice.

We may write down the tight-binding term that yields the potential term $H_{pq1}$. The additional terms are [5,6,17]

$$\Delta H = \frac{\lambda_{\Omega}}{3\sqrt{3}} \sum_{\langle i,j \rangle, \alpha \beta} \nu_{ij} \tau^i_\alpha \epsilon^j_\alpha \epsilon^{j_\beta},$$

$$-\ell E_z \sum_{i \alpha} t^i_\alpha \epsilon^i_\alpha \epsilon^{i_\alpha} \sigma_z \epsilon^{i_\alpha}, \quad (6)$$

The spin-valley dependent Dirac mass is given by

$$\Delta^\eta_z = \eta \lambda s \lambda_{SO} - \ell E_z + \eta \lambda \eta + s \Delta M. \quad (8)$$

It may be positive, negative or zero. The silicene system is described by the Hamiltonian $H + \Delta H$.

**Topological phases:** Any insulating state is characterized by a set of two topological quantum numbers $(C, C_s)$. Provided the spin $s_z$ is a good quantum number, they are given by $C = C^K + C^K_+ + C^K_-$ and $C_s = \frac{1}{2}(C^K + C^K_0 - C^K_1)$. $C^K_0$ is the summation of the Berry curvature in the momentum space over all occupied states of electrons with spin $s_z$ in the Dirac valley $K_p$, and calculated as $C^K_0 = \frac{g}{2} \text{sgn}(\Delta^\eta_z)$. All possible topological insulators are determined by the three parameters $E_z$, $\lambda_\Omega$ and $\Delta M$ with respect to $\lambda_{SO}$. Possible sets of topological numbers are $(0, 0), (2, 0), (0, \frac{1}{2}), (0, \frac{1}{2})$, up to the sign $\pm$. They are the trivial, QAH, QSH, SQAH insulators, respectively. Note that

**FIG. 1:** (Color online) Silicene nanoribbon in electric field. (a) It is decomposed into the device, right lead and left lead parts. The width is taken to be $W = 5$. (b) Silicene consists of the $A$-sublattice and the $B$-sublattice with layer separation $2\ell$. The energy of the $A$ sites (red disc) is lower than the one of the $B$ sites (blue disc) in electric field $E_z$. The edge mode is localized along the $A$ sites ($B$ sites) of the up (down) outmost edge of a nonoribbon. See Fig. 2 for the site-resolved DOS of the edge modes.

**FIG. 2:** (Color online) Band structure, DOS and conductance of zigzag silicene nanoribbons for (a) the QSH insulator phase, (b) the metallic phase at the phase transition point, and (c) the trivial insulator phase. These phases are obtained by applying electric field $E_z$. The phase transition occurs at $E_z = E_{cr}$. The number of bands is $2W + 2$ in the nanoribbon with width $W$. Here, the width is taken to be $W = 31$, and only a part of bands are shown. The band gap is degenerate (nongenerate) with respect to the up (red) and down (blue) spins at $E_z = 0$ ($E_z > 0$). Van Hove singularities emerge in the DOS at the points where the band dispersion is flat. The site-resolved DOS of the up-spin state at the outmost $A$ and $B$ sites of a nanoribbon are shown by red curves in the insets. There are finite DOS for the zero-energy edge states in the QSH insulator. The conductance is quantized by unit of $e^2/h$. 

where $t^i_\alpha = \pm 1$ for $i = A, B$. The Dirac Hamiltonian is

$$H_\eta = H_\eta^0 - \ell E_z \tau_z + \eta \lambda_\Omega \tau_z + \Delta M \sigma_z \tau_z, \quad (7)$$

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there are two types of trivial band insulators, which are the charge-density-wave (CDW) type insulator and the antiferromagnetic (AF) insulator.

A topological phase transition occurs when the band gap closes, or $\Delta^\eta_z = 0$. Let us review the topological phase transition along the $E_z$ axis, where the Dirac mass is given by $\Delta^\eta_z = \eta_\xi \lambda_{SO} - \ell E_z$. The condition $\Delta^\eta_z = 0$ implies $E_z = \pm E_{cr}$ with $E_{cr} = \lambda_{SO}/\ell$. It follows that $(C, C_z) = (0, 0)$ for $|E_z| < E_{cr}$ and $(0, \frac{1}{2})$ for $|E_z| > E_{cr}$. We have given the band structures at $E_z = 0$, $E_{cr}$, and $2E_{cr}$ in Fig 2. It is the characteristic feature known as the bulk-edge correspondence that zero-energy edge modes emerge in topological insulators with $(C, C_z) \neq (0, 0)$ and that these zero-energy edge modes are topologically protected against perturbation.

We may easily construct the phase diagrams by solving $\Delta^\eta_z = 0$. Those in the $(E_z, \Delta M)$ space and the $(E_z, \lambda_M)$ space are given in Figs 3 and 4 together with the pair of topological charges $(C, C_z)$, respectively. All possible topological insulators are found in these phase diagrams. The band structures at typical states are found in Figs 3 and 4 where the breakdown of the spin-valley symmetry is manifest. We proceed to characterize each phase by its characteristic pattern of the DOS and the conductance of a zigzag nanoribbon.

**DOS and conductance:** The natural framework for transport calculations in nanoscopic devices is the Landauer formalism. We consider a zigzag silicene nanoribbon divided into three regions [Fig 1]: the device region, the left lead and the right lead. The size of the device region is actually irrelevant due to the ballistic transport property.

In terms of single-particle Green’s functions, the low-bias conductance $\sigma(E)$ at the Fermi energy $E$ is given by

$$\sigma(E) = (e^2/h) \text{Tr} \left[ \Gamma_L(E) G_D(E) \Gamma_R(E) G_D(E) \right],$$

where $\Gamma_{LRi}(E) = i \left[ \Sigma_{LRi}(E) - \Sigma_{LR}^\eta(E) \right]$ with the self-energies $\Sigma_{LR}(E)$ and $\Sigma_{LR}^\eta(E)$, and

$$G_D(E) = \left[ E - H_D - \Sigma_{LR}(E) - \Sigma_{R}(E) \right]^{-1},$$

with the Hamiltonian $H_D$ for the device region. The self-energy $\Sigma_{LR}(E)$ describes the effect of the electrode on the electronic structure of the device, whose real part results in a shift of the device levels whereas the imaginary part provides a life time. It is to be calculated numerically.

The total density of states (DOS) reads

$$\rho(E) = -\pi^{-1} \text{Im} Tr G_D(E),$$

while the partial density of states at $i$ site reads

$$\rho_i(E) = -\pi^{-1} \text{Im} [G_D(E)_{ii}],$$

in terms of the Green function $G_D(E)$ of the device.

We have calculated the DOS $\rho(E)$ and the conductance $\sigma(E)$ of a nanoribbon as functions of the Fermi energy $E$, which is controlled by doping. We give the results at electric field $E_z = 0$, $E_{cr}$, and $2E_{cr}$ in Fig 4. A van Hove singularity occurs in the DOS at the point where the band dispersion is flat. As $E$ increases beyond the point, the Fermi level crosses a new band. A new channel opens and contributes to the conductance by $e^2/h$ for each spin and valley. It is clearly observed that the edge channel connects the tips of the Dirac cones with the same spin at the $K$ and $K'$ points.

We have also plotted the site-resolved DOS $\rho_i(E)$ of the up-spin states at the outmost $A$ and $B$ sites of a nanoribbon by red curves in the insets [Fig 2]. They represent degenerate zero-energy states at $E_z = 0$. As we have explained in Fig 1, the energy of the $A$ and $B$ sites become different for $E_z \neq 0$. It results in the downward (upward) shift of $\rho_{AB}(E)$ along the edge as $E_z$ increases. They are separated completely, and zero-energy states disappear for $E_z > E_{cr}$.

The zero-energy edge channel of a topological insulator is particularly important at half-filling, because it is topologically protected. We have calculated the conductance at half-filling by increasing the external field $E_z$ in the $(E_z, \Delta M)$
space and the \((E_z, \lambda_1)\) space. First, we increase \(E_z\) from \(E_z = 0\) at \(\Delta M = 0\), \(\lambda_{SO}\), \(\lambda_{SO}\) in the \((E_z, \Delta M)\) space [Fig.3]. Initially the conductance reads \(\sigma = 2e^2/h\) for \(\Delta M = 0\), where the system is in the QSH phase. It reads \(\sigma = e^2/h\), when the system is in the SQAH phase. Its band structure is shown in Fig.3(a), where the zero-energy edge states account for the conductance \(\sigma = e^2/h\). The conductance becomes zero as \(E_z\) increases and the system becomes the trivial AF insulator.

We confirm these observations by investigating the same problem in the \((E_z, \lambda_1)\) space [Fig.4]. The system is in the QAH phase for \(\lambda_1 > \lambda_{SO}\) at \(E_z = 0\), where \(\sigma = 2e^2/h\). We illustrate the band structure of the QSH insulator in Fig.4(b), where the zero-energy edge states account for the conductance \(\sigma = 2e^2/h\). The edge channel is helical (chiral) in the QSH (QAH) phase, but both of them transport the same amount of electric charges when the current is fed. We summarize the conductance in each topological insulator as in \((3)\).

**Field-effect topological quantum transistor:** The conductance is quantized in silicene nanoribbons. The simplest system is provided by applying electric field only\(2\), where quantized conductance changes from 2 to 0 at the critical electric field \(E_c\). This means the system acts as a transistor where “on” state can be switched off to “off” state by applying electric field. This transistor is “quantum” since the conductance is quantized, which is highly contrasted with the ordinal transistor, where the conductance is not quantized. Furthermore the conductance is topologically protected because the zero-energy edge state is topologically protected. Namely the conductance is robust against impurities due to its topological stability. Consequently we may call it a field-effect topological quantum transistor. This is the most energy-saving device since it utilizes the minimum conductance.

We are able to design a three-digit quantum transistor by attaching antiferromagnet. Namely the conductance changes in three steps 2, 1, 0 with increasing electric field when \(|\Delta M| < \lambda_{SO}\). When \(|\Delta M| > \lambda_{SO}\), the conductance changes in three step 0, 1, 0. It acts as a three-step transistor, where the system is first in the “off” state, then become “on” state and finally become “off” state with the increase of electric field.

**Conclusions:** We have analyzed the DOS and the conductance in silicene nanoribbons. There are finite DOS due to the zero-energy edge states in the topological phase, while they disappear in the trivial phase [Fig.2]. Local DOS measurement is a direct evidence of the existence of the edge states, which can be achieved by spatially resolved STM/STS. This must be the most efficient way to make an experimental observation of a topological phase transition. Furthermore we can determine the band gap by measuring the DOS. A precise measurement is possible owing to the van-Hove singularities present at the tips of the conduction and valence bands [Fig.2].

Conductance measurement is also a direct method to observe a topological phase transition. We have proposed a field-effect topological quantum transistor with the use of the zero-energy edge state of a silicene nanoribbon. This could be a basic component of future topological quantum devices.

In passing we address the problem how narrow the nanoribbon can be. The penetration depth of the zero-energy edge state has already been shown to be as short as the atomic scale\(2\) in zigzag nanoribbons. Hence we may use a quite narrow nanoribbon to detect and make use of the topological properties of silicene.

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