Monolayer Topological Insulators: Silicene, Germanene and Stanene

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We report the recent progress on the theoretical aspects of monolayer topological insulators including silicene, germanene and stanene, which are monolayer honeycomb structures of silicon, germanium and tin, respectively. They show quantum spin Hall effects in nature due to the spin orbit interaction. The band gap can be tuned by applying perpendicular electric field, which induces a topological phase transition. We also analyze the topological properties of generic honeycomb systems together with the classification of topological insulators. Phase diagram of topological insulators and superconductors in honeycomb systems are explicitly determined. We also investigate topological electronics including a topological field-effect transistor, the topological Kirchhoff’s law and the topological spin-valleytronics.

I. INTRODUCTION

Monolayer materials are one of the most active fields of condensed matter physics. Graphene, monolayer honeycomb structure of carbon atoms, is the first experimentally realized monolayer material. Its low-energy band structure is described by the Dirac theory, which results in various novel physical properties. The success of graphene evokes an extensive search for other monolayer materials. In particular, monolayer topological materials are fascinating, realizing topological insulators and topological superconductors.

A natural question is whether other monolayer honeycomb systems purely made of one kind of atoms are possible. It is shown that monolayer honeycomb systems made of silicon, germanium and tin are possible, which are named silicene, germanene and stanene, respectively. Silicene is named after the combination of silicon and suffix "ene", which means the sp bonding structure. Germanene is also named after germanium + "ene". Stanene is named after the Latin word "stannum" for tin.

Silicene, Germanene and stanene are expected to be topological insulators. Topological insulator (TI) is a distinctive state of matter indexed by topological numbers, and characterized by an insulating gap in the bulk accompanied by topologically protected gapless edges. Thus the physics of these materials is located at the confluence of graphene and topological insulators, which results in very rich physics.

Silicene and germanene are proposed by first-principles calculations, where their stability and the emergence of the Dirac cone are predicted by first-principles calculations. It is shown that the band gap of silicene is electrically controllable by applying perpendicular electric field to silicene plane by the first-principle calculations and based on the Dirac theory. A first-principles calculation shows that the Dirac cones are hidden in silicene fabricated on the Ag substrate due to the strong hybridization between silicene and Ag substrate.

First suggestive observations of silicene were reported in 2010. Silicene has been grown on various substrates such as the Ag substrate and the ZrB$_2$ substrate, the Ir substrate and the MoS$_2$ substrate. Germanene is synthesized on the Au substrate and Pt substrate. There are several experiments on silicene. In particular, silicene was demonstrated in 2015 to act as a field-effect transistor at room temperature. There are reviews on experimental aspects of silicene.

There are several proposal on realizing free-standing like silicene on substrates by first-principles calculations. Silicene will be grown on graphene, hexagonal boron-nitride, hydrogen-processed Si(111) surface, hydrogen-processed Ge(111) surface, Cl-passivated Si(111) and clean CaF$_2$(111) surfaces, solid argon, between bilayer graphene and intercalating alkali metal atoms between silicene and the metal substrate.

II. GRAPHENE AND SILICENE

The basic structure of graphene and silicene is a honeycomb lattice generated by the fundamental translational vectors $\alpha_1$ and $\alpha_2$. It consists of two triangular sublattices made of inequivalent lattice sites $A$ and $B$ [Fig. 1(a)]. The reciprocal lattice is also a honeycomb lattice. A dotted rectangular represents a unit cell, which contains two inequivalent points $K$ and $K'$.

![Image](image_url)

FIG. 1: (a) The honeycomb structure, made of two fundamental vectors $\alpha_1$ and $\alpha_2$, consists of two sublattices made of $A$ and $B$ sites. A dotted rectangular represents a unit cell. (b) The reciprocal lattice is also a honeycomb lattice. A dotted rectangular represents a unit cell, which contains two inequivalent points $K$ and $K'$.

A. Graphene

Graphene is described by the simplest tight-binding model on a honeycomb lattice [Fig. 2].

$$\hat{H}_0 = -t \sum_{\langle i,j \rangle s} c_{is}^\dagger c_{js},$$

(2.1)
The energy spectrum is obtained as
\[ E(k) = t \sqrt{1 + 4 \cos \frac{ak_x}{2} \cos \frac{\sqrt{3}ak_y}{2} + 4 \cos^2 \frac{ak_x}{2}}. \]

The gap closes at the \( K_\eta \) point defined by
\[ K_\eta = \frac{1}{a} \left( \frac{4\pi}{3}, \frac{2\pi}{3} \right) \quad \text{with} \quad \eta = \pm. \]

The \( K_+ \) and \( K_- \) points are identical to the \( K \) and \( K' \) points, respectively. Because the dispersion relation is linear for \( k_i \approx 0 \), they are also called the Dirac points. See Figs. 2 and 3.

In the vicinity of the \( K_\eta \) point, the Hamiltonian is approximated by
\[ \hat{H}_\eta = \sum_{ij} \int d^2k \left( c_{\eta A,s}^\dagger, c_{\eta B,s}^\dagger \right) H_{\eta s}^c \left( c_{\eta A,s}, c_{\eta B,s} \right), \]
with
\[ H_{\eta s}^c = \hbar v_F \left( \eta k_x \tau_x + k_y \tau_y \right) = \hbar v_F \begin{pmatrix} 0 & \eta k_x - i k_y \\ \eta k_x + i k_y & 0 \end{pmatrix}, \]
where \( \tau = (\tau_x, \tau_y, \tau_z) \) is the Pauli matrix of the sublattice pseudospin for the \( A \) and \( B \) sites, and \( v_F = \sqrt{3} a t \) is the Fermi velocity with \( a \) being the lattice constant. The dispersion relation is linear for \( k_i \approx 0 \). We refer to \( H_{\eta}^c \) as the Dirac Hamiltonian at the Dirac point \( K_\eta \).

The basic nature of silicene is described also by the tight-binding model \((2.1)\). There are two additional features making silicene essentially different from graphene. One is the presence of the spin-orbit interaction, which makes silicene a topological insulator\([22]\). The other is its buckled structure with a layer separation between the two sublattices \([22][23]\). This freedom allows us to tune the gap by introducing a potential difference between the two sublattices \([22][23]\). When we apply electric field \( E_z \) perpendicular to silicene, the tight-binding Hamiltonian reads
\[ \hat{H} = -i \sum_{(ij),s} c_{is}^\dagger c_{js} + i \frac{\lambda_{SO}}{3\sqrt{3}} \sum_{(ij),s} s \nu_{ij} c_{is}^\dagger c_{js} - i \sum_{is} \mu_i E_z c_{is}^\dagger c_{is}, \]
where \( \{(i,j)\} \) run over all the next-nearest neighbor hopping sites. The spin index stands for \( s = \uparrow, \downarrow \) for indices and for \( s = \pm \) within equations. It describes germaine and stanene as well.

We explain each term. (i) The first term represents the usual nearest-neighbor hopping with the transfer energy \( t \). (ii) The second term represents the effective SO coupling with \( \lambda_{SO} \), where \( \nu_{ij} = +1 \) if the next-nearest-neighboring hopping is anticlockwise and \( \nu_{ij} = -1 \) if it is clockwise with respect to the positive \( z \) axis\([25]\). (iii) The third term represents the staggered sublattice potential with \( \mu_i = +1 (1) \) for the \( A (B) \) site\([26]\). Explicit values of these parameters are summarized in the Table \([1] \). By diagonalizing the Hamiltonian by setting \( E_z = 0 \), we obtain the band structure illustrate as in Fig. 3(b2).

The prominent feature is that the gap is open due to the SO interaction, and hence silicene is an insulator. A large SO interaction with \( \lambda_{SO} = 0.3 \text{eV} \) is materialized in functionalized...
where $|v_F|$ is the unit of $10^3$ m/s, and $\lambda_{SO}$ in the unit of meV. $\lambda_R$ is the Rashba SO interaction strength in the unit of meV. See (7.1). $\ell$ is the buckle height, while $\theta$ is the bond angle. Taken from Ref.[42].

|         | $t$(eV) | $v$ | $a$(Å) | $\lambda_{SO}$ | $\lambda_R$ | $\ell$ | $\theta$ |
|---------|---------|-----|--------|----------------|-------------|--------|--------|
| Graphene| 2.8     | 9.8 | 2.46   | 10^{-3}        | 0           | 0      | 90     |
| Silicene| 1.6     | 5.5 | 3.86   | 3.9            | 0.7         | 0.23   | 101.7  |
| Germanene| 1.3    | 4.6 | 4.02   | 43             | 0.107       | 0.73   | 106.5  |
| Stanene | 1.3     | 4.9 | 4.70   | 43             | 9.5         | 0.33   | 107.1  |

TABLE I: The parameters charactering graphene, silicene and germanene. Here, $v_F$ is in the unit of $10^3$ m/s, and $\lambda_{SO}$ in the unit of meV. $\lambda_R$ is the Rashba SO interaction strength in the unit of meV. See (7.1). $\ell$ is the buckle height, while $\theta$ is the bond angle. Taken from Ref.[42].

FIG. 4: Electrically tunable band gap and topological phase transition of silicene. Silicene is a QSH insulator without electric field. By applying electric field, the band gap reduces and closes at the critical electric field $\pm E_{cr}$. Above the critical electric field, silicene becomes a QVH insulator.

Stanene[21], which will be a topological insulator at room temperature.

The low-energy physics near the Fermi energy is described by the Dirac theory, which is constructed just as in the case of graphene. We rewrite the Hamiltonian (2.8) in the form of (2.6). The Dirac Hamiltonian is explicitly given by

$$H_s^\eta = \begin{pmatrix} \Delta_s^\eta & \hbar v_F (\eta k_x - i k_y) \\ \hbar v_F (\eta k_x + i k_y) & -\Delta_s^\eta \end{pmatrix},$$

where

$$\Delta_s^\eta = \eta s \lambda_{SO} - \ell E_z \equiv -\ell (E_z - \eta s E_{cr}),$$

with

$$E_{cr} \equiv \lambda_{SO}/\ell.$$  

Note that $\Delta_s^\eta$ acts as the Dirac mass. The energy spectrum reads

$$E(k) = \pm \sqrt{\hbar v_F k^2 + (\Delta_s^\eta)^2}.  \hspace{0.5cm} (2.12)$$

The gap is given by $2|\Delta_s^\eta| = 2\ell (|E_z| - \eta s E_{cr})$.

It is important that the band gap is tunable by controlling external electric field $E_z$. The gap is open when $E_z = 0$. As $|E_z|$ increases, the gap become narrower [Fig.4], and it closes at $E_z = \eta s E_{cr}$, where silicene is semimetallic just as in graphene. As $|E_z|$ increases further, the gap opens again.

C. Generalized Dirac mass terms

There are actually other ways to control the band gap by introducing other interactions to silicene. Since each Dirac cone is indexed by two parameters $\eta = \pm$ and $s = \pm$, the most general Dirac mass must have the following expression,

$$\Delta_s^\eta = \eta s \lambda_{SO} - \eta \lambda_V + \eta \lambda_H + s \lambda_{SX},$$  

so that it has four independent parameters, $\lambda_{SO}$, $\lambda_V$, $\lambda_H$ and $\lambda_{SX}$. We have already discussed the first two terms representing the SO interaction and the sublattice staggered potential with $\lambda_V = \ell E_z$. We may write down the tight-binding terms that yield the fourth and fifth terms[42],

$$\frac{i}{3} \lambda_h \sum_{\langle{i,j}\rangle s} \nu_{ij} c_i^\dagger c_j, \lambda_{SX} \sum_{is} s \mu_i c_i^\dagger c_i.$$  

(2.14)

The fourth term describes the Haldane interaction induced by the photo-irradiation, where $\lambda_{SO} = \hbar v_F A^2 \Omega^{-1}$ with $\Omega$ the frequency and $A$ the dimensionless intensity[42,50]. The fifth term describes the antiferromagnetic exchange magnetization[43].

Here we note that there are a variety of 2D materials whose low-energy physics is described by the Dirac Hamiltonian (2.9) with the Dirac mass (2.13). We call them general honeycomb systems. Examples are monolayer antiferromagnetic manganese chalcogenophosphates (MnP$X_3$, X = S, Se)[51] and perovskite G-type antiferromagnetic insulators grown along [111] direction[52].

In what follows we analyze the Dirac Hamiltonian (2.9) with the Dirac mass (2.13). It can be positive, negative or zero. The band gap is given by $2|\Delta_s^\eta|$.

III. TOPOLOGICAL PHASE TRANSITION

A. Chern numbers

For any insulating state $|\psi(k)\rangle$ we may define a "gauge potential" in the momentum space by

$$a_k(k) = -i \langle \psi(k) | \partial_k | \psi(k) \rangle,$$  

(3.1)
which is properly called the Berry connection. Then we may define the "magnetic field" in the momentum space, which is properly called the Berry curvature $F(k)$,

$$F(k) = \frac{\partial}{\partial k_x} a_y(k) - \frac{\partial}{\partial k_y} a_x(k).$$  \hfill (3.2)

The Chern number is the integral of the Berry curvature $F(k)$ over the first Brillouin zone, which is the total "magnetic flux",

$$C = \frac{1}{2\pi} \int d^2 k F(k).$$  \hfill (3.3)

We have calculated the Berry curvature with the use of the tight-binding Hamiltonian (3.8), which we illustrate in Fig.5. The Berry curvature is strictly localized at the $K$ and $\tilde{K}$ points. This feature remains unchanged even if we include the extra terms (2.14). Consequently, the Dirac Hamiltonian is valid to make a topological analysis to each valley, which is indexed by the spin $s = \uparrow, \downarrow$ and the valley index $\eta = \pm$. Namely, it is possible to assign the Chern number $C_\eta^s$ to each valley.

When the Hamiltonian is given by (2.9), the Berry curvature is explicitly calculated for each valley as

$$F^\eta_s(k) = -\eta \frac{\Delta^\eta_s}{2 (h v_F k)^2 + (\Delta^\eta_s)^2}.$$  \hfill (3.4)

The Chern number is obtained as

$$C_\eta^s = -\frac{\eta}{2} \text{sign}(\Delta^\eta_s),$$  \hfill (3.5)

where the Dirac mass $\Delta^\eta_s$ is given by (2.13).

The Chern number is quantized as $C_\eta^s = \pm \frac{1}{2}$. It is insensitive to a deformation of the band structure provided the gap is open. On the other hand, it changes its sign as the Dirac mass $\Delta^\eta_s$ changes its sign. Such a quantity is a topological charge. Hence an insulator phase is indexed by a set of four Chern numbers $C_\eta^s$. A topological phase transition occurs when the sign of the Dirac mass $\Delta^\eta_s$ changes.

It is instructive to make a reinterpretation of the Chern number $C_\eta^s$. When the Hamiltonian is given in terms of the $2 \times 2$ Hamiltonian as in (2.9), or $H^\eta_s = \tau \cdot d$ with $d_x = \eta h v_F k_x$, $d_y = \eta h v_F k_y$, $d_z = \Delta^\eta_s$, the Chern number $C_\eta^s$ is equivalent to the Pontryagin number,

$$C_\eta^s = \frac{1}{4\pi} \int d^2 k \left( \frac{\partial d}{\partial k_x} \times \frac{\partial d}{\partial k_y} \right) \cdot d.$$  \hfill (3.6)

The Pontryagin number is a topological number which counts what times the vector $\hat{d}$ wraps a sphere. We use the polar coordinate of the $\hat{d}$ vector, $\hat{d} \pm i \hat{d} = \sqrt{1 - \sigma^2(k)} e^{i \varphi}$, $\hat{d} = \sigma(k)$, and we obtain

$$C_\eta^s = \frac{\eta}{4\pi} \int d^2 k \varepsilon_{ij} \sigma_i \sigma_j \theta = -\frac{\eta}{2} \int_0^1 d\sigma,$$  \hfill (3.7)

which agrees with (3.5). The pseudospin texture forms a meron structure in the momentum space. A meron is a topological structure which has a half integer Pontryagin number as shown in Fig.5.

![FIG. 6: Illustration of a meron structure in momentum space. A meron with the Pontryagin number (a) $1/2$, which core spin is pointing up direction, (b) $-1/2$, which core spin is pointing down direction.](image)

**B. Classification of topological insulators**

We have defined four Chern numbers $C_\eta^s$. Equivalently we may define the total Chern number $C$, the spin Chern number $C_\eta$, the valley Chern number $C^V$, and the spin-valley Chern number $C^{sV}$,

$$C = C_{\uparrow}^\eta + C_{\downarrow}^\eta + C_{\uparrow}^V + C_{\downarrow}^V,$$  \hfill (3.8)

$$C_{\eta} = \frac{1}{2} (C_{\uparrow}^\eta + C_{\downarrow}^\eta - C_{\downarrow}^\eta - C_{\uparrow}^\eta),$$  \hfill (3.9)

$$C_{v} = C_\uparrow^V - C_{\downarrow}^V + C_{\downarrow}^V - C_{\uparrow}^V,$$  \hfill (3.10)

$$C_{sv} = \frac{1}{2} (C_{\uparrow}^V - C_{\downarrow}^V - C_{\downarrow}^V + C_{\uparrow}^V).$$  \hfill (3.11)

We make an important comment. The valley Chern number and the spin-valley Chern number are well defined only in the Dirac theory. Namely they are ill defined in the tight-binding model. Hence, we may call $C$ and $C_{\eta}$ the genuine Chern numbers.

Possible sets of genuine Chern numbers $(C,C_{\eta})$ are $(0,0),(2,0),(0,1),(1,1/2)$ up to the sign $\pm$. They are the trivial, quantum anomalous Hall (QAH), quantum spin Hall (QSH), spin-polarized quantum anomalous Hall (SQAH) insulators, respectively. Note that there are two-types of trival band insulators, which are quantum valley Hall (QVH) insulator$^{87,89}$ and quantum spin-valley Hall (QSVH) insulator with antiferromagnetic (AF) order$^{90}$.

We comment on the relation between the $Z_2$ index and the spin Chern number. The spin Chern number $C_{\eta}$ is identical to the $Z_2$ index by modulo 2 when there exists the time-reversal symmetry$^{31}$. The spin Chern number is well defined even when there is no time-reversal symmetry, while the $Z_2$ index is well defined even when $s_z$ is not a good quantum number.

**IV. TOPOLOGICAL EDGE**

**A. Bulk-edge correspondence**

The most convenient way to determine if the system is topological or trivial is to employ the bulk-edge correspondence. When there are two topological distinct phases, a topological phase transition must occur between them. It is generally accepted that the band gap must close at the topological phase transition point since the topological number cannot change.
Second, the spin degeneracy is resolved due to the SO interaction. We have shown up(down)-spin band in magenta(cyan) sites while the other of sites have higher energy. This property enables us to identify the edge modes occurring in the upper or lower edges. Hence there are 16 states indexed by them. The genuine topological numbers are only \( C_s \) and \( C_v \).

### Table II: Corresponding to the spin and valley degrees of freedom, there are 4 Chern numbers \( C_{sv}^s, \) each of which takes \( \pm \frac{1}{2} \). Equivalently they are given by the Chern, spin Chern, valley Chern and spin-valley Chern numbers \( C, C_s, C_v \) and \( C_{sv} \). They are independently controlled by the four parameters \( \lambda_{SO}, \lambda_V, \lambda_M \) and \( \lambda_{SX} \). Hence there are 16 states indexed by them. The genuine topological numbers are only \( C \) and \( C_v \).

|       | \( C^s \) | \( C^{s'} \) | \( C^v \) | \( C^{v'} \) | \( C \) | \( 2C_s \) | \( 2C_v \) | \( 2C_{sv} \) |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| QAH   | \( \frac{1}{2} \) | \( \frac{1}{2} \) | \( \frac{1}{2} \) | \( \frac{1}{2} \) | 2          | 0          | 0          | 0          |
| SQAH  | \( \frac{1}{2} \) | \( \frac{1}{2} \) | \( \frac{1}{2} \) | \( \frac{1}{2} \) | 1          | 1          | 1          | \(-1\)     |
| SQUH  | \( \frac{1}{2} \) | \( -\frac{1}{2} \) | \( \frac{1}{2} \) | \( \frac{1}{2} \) | 1          | \(-1\)     | 1          | 1          |
| QVH   | \( \frac{1}{2} \) | \( \frac{1}{2} \) | \( -\frac{1}{2} \) | 0          | 1          | 2          | 0          | 0          |
| QSH   | \( \frac{1}{2} \) | \( \frac{1}{2} \) | \( \frac{1}{2} \) | \( \frac{1}{2} \) | 1          | 1          | \(-1\)     | \(-1\)     |
| QSVH  | \( \frac{1}{2} \) | \( \frac{1}{2} \) | \( \frac{1}{2} \) | \( \frac{1}{2} \) | 0          | 0          | 0          | \(-2\)     |
| QSH   | \( -\frac{1}{2} \) | \( -\frac{1}{2} \) | \( -\frac{1}{2} \) | \( \frac{1}{2} \) | 0          | \(-2\)     | 0          | 0          |
| QSVH  | \( -\frac{1}{2} \) | \( -\frac{1}{2} \) | \( -\frac{1}{2} \) | \( \frac{1}{2} \) | 1          | \(-1\)     | \(-1\)     | \(-1\)     |
| SQAH  | \( -\frac{1}{2} \) | \( -\frac{1}{2} \) | \( -\frac{1}{2} \) | \( \frac{1}{2} \) | 0          | 0          | \(-2\)     | 0          |

When a nanoribbon has only the valley Chern number and the spin-valley Chern number, no edge modes emerge because these numbers are not defined in the vacuum. Nevertheless these numbers are also topological numbers within the bulk.

We may also analyze a silicene nanoribbon in the QAH phase. The band structure is given by Fig. 7 (b1), where we have applied week electric field \( E_z \) to resolve the degeneracy. The spin and the current direction are shown in both edges in Fig. 7 (b2). The edge current does not convey spins. Such an edge is called a chiral edge.

### C. Inner edges

When a nanoribbon has only the valley Chern number and the spin-valley Chern number, no edge modes emerge because these numbers are not defined in the vacuum. Nevertheless these numbers are also topological numbers within the bulk. We may consider a junction separating two different topological phases in a single honeycomb system. We call such a junction an inner edge. In contrast we may call a real edge of a nanoribbon an outer edge. There is a crucial difference between gapless edge modes appearing along an inner edge and an outer edge. Any gapped state is indexed by a set of four topological numbers \( \{ C, C_s, C_v, C_{sv}\} \). Consequently, an inner edge state carries a gapless edge mode indexed by the difference \( \Delta C, \Delta C_s, \Delta C_v, \Delta C_{sv} \) between the two adjacent gapped states. More precisely, we set \( \Delta C = C^L - C^R \) and so on, when the topological insulator with \( \{ C^L, C^s_s, C^L_v, C^L_{sv}\} \) is on the left-hand side of the one with \( \{ C^R, C^R_s, C^R_v, C^R_{sv}\} \). On the other hand, an outer edge state can carry a gapless edge mode that may resolve the degeneracy by applying weak electric field. See Table II.
mode only indexed by \((C, C_s)\) of the gapped state because the valley Chern numbers are ill defined in the vacuum.

We illustrate a nanoribbon which contains the QSH and QVH phases in Fig. 8, where there are two outer edges and one inner edge. As we have argued, the outer edge of the QSH part is helical, while the outer edge of the QVH part has no gapless edge modes. The nature of the inner edge is seen by analyzing the band structure in Fig. 8(b). It contains only four nondegenerate gapless states. On one hand, two solid lines correspond to the helical edge between the QSH part and the vacuum. On the other hand, two dotted lines correspond to the inner edge between the QSH and QVH parts, which is also helical. It should be noted that the inner edge modes cross the Fermi energy at the \(K\) and \(K'\) points.

D. Topological Kirchhoff law

We consider a configuration where three different topological insulators meet at one point: See Fig. 9. In this configuration there are three edges forming a Y-junction. The condition which edges can make a Y-junction is the conservation of these topological numbers at the junction. This law is a reminiscence of the Kirchhoff law, which dictates the conservation of currents at the junction of electronic circuits. We call it the topological Kirchhoff law [36].

We present an interesting interpretation of the topological Kirchhoff law. We may regard each topological edge state as a world line of a particle carrying the four topological charges. The Y-junction may be interpreted as a scattering process of these particles. In this scattering process, the topological charges conserve. We have shown that we can control the mass of Dirac cones with the spin and valley independently in silicene. Our findings will open a new way to topological spin-valleytronics, where the spin and valley degrees of freedom and the topology are fully manipulated.
B. Circular geometry

We consider a cylindrical symmetric domain with the radius \( r_0 \) at the origin of the \( xy \) plane. A phase transition occurs at \( r = r_0 \), where \( \Delta_0^2(r) = 0 \). The equation of motion \( \mathcal{H}_K \psi = 0 \) reads

\[
\Delta_0^2(r) \psi_{s,A}^0 + \hbar v_F e^{i\eta \theta} \left( i \partial_r - \frac{1}{r} \partial_\theta \right) \psi_{s,B}^0 = 0,
\]

\[
\hbar v_F e^{-i\eta \theta} \left( i \partial_r + \frac{1}{r} \partial_\theta \right) \psi_{s,A}^0 - \Delta_0^2(r) \psi_{s,B}^0 = 0. \tag{5.4}
\]

We can solve this for zero-energy states as

\[
\psi_{s,A}^0(r, \theta) = \frac{C}{\sqrt{r}} e^{i\eta \theta/2} \exp \left[ \frac{\xi}{\hbar v_F} \int_0^r \Delta_0^2(r) \, dr' \right], \tag{5.5}
\]

and \( \psi_{s,B}^0(r, \theta) = i \zeta \psi_{s,A}^0(r, \theta) \), where \( C \) is the normalization constant and \( \zeta = \pm 1 \). The sign of \( \zeta \) is determined so as to make the wave function finite in the limit \( r \to \infty \).

C. Interface induced by electric field

We apply an inhomogeneous electric field,

\[
\Delta_0^2(r) = \lambda_{SO} - \lambda_V (r) \tag{5.6}
\]

with \( \lambda_V (r) = \ell E_z (r) > \lambda_{SO} \) for \( r < r_0 \). The region \( r < r_0 \) is a trivial insulator, while the region \( r > r_0 \) is a quantum spin-Hall insulator. The zero-energy helical edge current flows along the circle \( r = r_0 \).

VI. TOPOLOGICAL QUANTUM FIELD-EFFECT TRANSISTOR

We next calculate the conductance of a nanoribbon by using the Landauer formalism\[\text{[52,53]}\]. The conductance is quantized in silicene nanoribbons. Indeed, one channel has a quantized conductance \( e^2/h \). Accordingly, the conductance is obtained by counting the number of bands. We show the conductance in Fig.10. When electric field is not applied, there are helical edge states, which contribute to the conductance \( 2e^2/h \) since up and down spin channels contribute to the conductance. When the electric field \( E_z \) exceeds the critical value \( E_{z_{\text{cr}}} \), the edge states disappear since the nanoribbon becomes a trivial insulator, which results in zero conductance. This means the system acts as a transistor where the "on" state can be switched to the "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\[\text{[26]}\]. This is the most energy-saving device since it utilizes the minimum conductance.

We have calculated the density of states (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 \( E_z = 0, E_{z_{\text{cr}}} \) and \( 2E_{z_{\text{cr}}} \) in Fig.10. 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 tops of the Dirac cones with the same spin at the \( K \) and \( K' \) points.

We have also plotted the site-resolved DOS \( \rho_s(E) \) of the up-spin states at the outmost \( A \) and \( B \) sites of a nanoribbon by red curves in the insets [Fig.10]. They represent degenerate zero-energy states at \( E_z = 0 \). As we have explained in Fig.7, the energy of the \( A \) and \( B \) sites become different for \( E_z \neq 0 \). It results in the downward (upward) shift of \( \rho_s(A,B)(E) \) along the edge as \( E_z \) increases. They are separated completely, and zero-energy states disappear for \( E_z > E_{z_{\text{cr}}} \).
VII. QUANTUM ANOMALOUS HALL EFFECTS

Silicene has an additional interaction term, which we have so far neglected. It is the Rashba SO interaction given by

\[ -\frac{i}{3} \lambda_R \sum_{\langle i,j \rangle, \alpha \beta} \mu_i c_{i\alpha}^\dagger \left( \mathbf{\sigma} \times \mathbf{d}_{ij} \right)_{\alpha \beta} c_{j\beta} \]  

(7.1)

in the tight-binding model. Here, \( \lambda_R \) represents the Rashba SO coupling strength associated with next-nearest neighbor hopping, where \( \mu_i = \pm 1 \) for the A (B) site, and \( \mathbf{d}_{ij} = \mathbf{d}_{ij} / |\mathbf{d}_{ij}| \) with the vector \( \mathbf{d}_{ij} \) connecting two sites \( i \) and \( j \) in the same sublattice:\(^{65}\) The Dirac theory of the Rashba term is given by

\[ \eta \tau_z a \lambda_R \left( k_y \sigma_x - k_x \sigma_y \right). \]  

(7.2)

The Rashba term vanishes at the \( K \) and \( K' \) points. Hence the Rashba interaction is negligible as far as the low-energy physics near the Dirac points is concerned.

There exists an exceptional case in which we cannot neglect the Rashba interaction. We have previously studied the interaction term\(^{(2.13)}\) affecting the Dirac mass. There is another type of interactions, which do not contribute to the Dirac mass but shift the bands into the opposite directions between up and down spins. The most important one is given by the exchange interaction,

\[ M \sum_{is} s c_i^\dagger \sigma_z c_i \quad \text{or} \quad M \sigma_z \]  

(7.3)

in the tight-binding model or in the Dirac theory. We show the band structure of a nanoribbon with the exchange interaction in Fig.11\(\text{a)\). We see that the two Dirac cones with the opposite spins approach as \( |M| \) increases and touch each other at \( |M| = \lambda_{SO} \). Then, we expect naively the level crossing to occur for \( |M| > \lambda_{SO} \), that is, the two Dirac cones to penetrate into each other. Actually, the level crossing turns into the level anticrossing due to the spin mixing caused by the Rashba interaction \( \lambda_R \). The new phase is the QAH insulator\(^{63}\) with the Chern number 2. We show the Berry curvature in Fig.11\(\text{b)}\), where it takes a large value where the bands almost touch the Fermi energy away from the \( K \) and \( K' \) points. The spin direction is inverted and the spin forms a skyrmion texture, which results in the Chern number 1. The total Chern number is 2 since there are two skyrmions at the \( K \) and \( K' \) points.

VIII. SYMMETRY PROTECTED TOPOLOGICAL CHARGE

The Chern number \( \mathcal{C} \) is always quantized. However, the other ones \( \mathcal{C}_i \) are not so when the relevant symmetry is broken. Indeed, the spin \( s_z \) symmetry is broken by the Rashba interaction. We here analyze this problem.

There exists an alternative expression for the Chern number in terms of the Green function\(^{63}\). It reads

\[ \mathcal{C} = \frac{\varepsilon_{\alpha \beta \gamma}}{6} \int \frac{d^2k}{(2\pi)^2} \int_{-\infty}^{\infty} d\omega \]

\[ \times \text{Tr}[G\partial_{k_\alpha} G^{-1}G\partial_{k_\beta} G^{-1}G\partial_{k_\gamma} G^{-1}], \]  

(8.1)

with \( i = s, v, sv \) together with \( \chi_s = \sigma_z, \chi_v = \eta_z, \chi_{sv} = \sigma_z \eta_z \). Provided the spin \( \sigma_z \) and the pseudospin \( \eta_z \) are good quantum numbers, namely, \([H, \sigma_z] = [H, \eta_z] = 0\), we are able to prove that these are identical to\(^{72, 73}\) and\(^{39}\) by following the method\(^{73}\). We may use the formula\(^{63}\) even if symmetries are broken. They are no longer quantized when the symmetries are broken. Accordingly, we call them symmetry protected topological charges.

In the presence of the Rashba interaction, the spin Chern number is explicitly calculated as

\[ \tilde{\mathcal{C}}_s = \frac{\mathcal{C}_s}{1 + (a\lambda_R / \nu_F)^2}, \]

where \( \mathcal{C}_s \) is the spin Chern number without the Rashba interaction. This yields \( \tilde{\mathcal{C}}_s = 1 - 5.9 \times 10^{-7} \), where we have used \( \nu_F = 5.5 \times 10^5 \text{m/s}, a = 3.86 \text{Å} \) and \( \lambda_R = 0.7 \text{meV} \) as sample parameters of silicene. Surely \( \tilde{\mathcal{C}}_s \) is not quantized, but the deviation is negligibly small. Furthermore, we can check that the edge mode remains practically gapless. The spin mixing can be neglected in practical purposes.
IX. TOPOLOGICAL SUPERCONDUCTOR

Topological superconductors are superconductors which have nontrivial topological numbers. The bulk band spectrum has a full gap due to the superconducting gap, while the edge states appear at the sample of edges as in the case of topological insulators. An intriguing feature is that these edge states support Majorana fermions.

A. Majorana fermion

Majorana fermion is one of the hottest topics in the condensed matter physics. Majorana fermion operator $\gamma$ satisfies the anti-commutation relation $\{\gamma, \gamma^\dagger\} = 1$ and the Majorana condition $\gamma = \gamma^\dagger$, indicating that a Majorana fermion is a particle which is its own anti-particle.

In the BCS theory, superconductor is expressed by the Bogoliubov–de Gennes (BdG) Hamiltonian,

$$ H = \frac{1}{2} \sum_k \left( c_{k}^\dagger, c_{-k} \right) H_{BdG}(k) \left( c_{k}, c_{-k}^\dagger \right), \tag{9.1} $$

based on the Nambu representation $\left( c_{k}, c_{-k}^\dagger \right)$, which is a combination of the particle and hole operators. The BdG Hamiltonian has a particle-hole symmetry,

$$ \Xi H_{BdG} \Xi^{-1} = -H_{BdG}, \tag{9.2} $$

with respect to the particle-hole operator $\Xi$ satisfying $\Xi^2 = 1$. The states with the energy $E$ and $-E$ are to be identified in the Nambu representation. The creation and annihilation operators of these two states satisfy $\gamma^E = \gamma_{-E}$. Consequently, we obtain $\gamma_0^\dagger = \gamma_0$ for a single zero-energy state ($E = 0$) if there is such one. As a result, a single zero-energy state with the particle-hole symmetry is a Majorana fermion.

B. Topological superconductor in honeycomb system

A topological superconductor is obtained from a QAH insulator by attaching an $s$-wave superconductor to $t_j^{[2]}$. Indeed, Cooper pairs are formed between up and down spins at the same site of the honeycomb system. The resultant BCS Hamiltonian reads $H_{BCS} = H_K + H_K^* + H_{SC}$ with

$$ H_{SC} = \sum_{\tau=A,B} \left[ \Delta_{SC} c_{\tau \uparrow}^K \left( k \right) c_{\tau \downarrow}^{K^\dagger} \left( -k \right) + \Delta_{SC} c_{\tau \downarrow}^K \left( k \right) c_{\tau \uparrow}^{K^\dagger} \left( -k \right) \right] + \text{h.c.} \tag{9.3} $$

in the momentum representation, where $\Delta_{SC}$ is the superconducting gap. A finite gap present in a superconducting state allows us to evaluate the Chern number of the state to determine whether it is topological. Alternatively we may examine the emergence of gapless edge modes by calculating the band structure of a nanoribbon with zigzag edge geometry based on this Hamiltonian. The BCS Hamiltonian is rewritten into the BdG Hamiltonian,

$$ H_{BdG} = \begin{pmatrix} H_K \left( k \right) & H_\Delta \\ H_\Delta^\dagger & -H_{K^*}^\dagger \left( -k \right) \end{pmatrix}, \tag{9.4} $$

by introducing the Nambu representation for the basis vector, i.e., $\Psi = \{ \psi_{\uparrow A}, \psi_{\downarrow A}, \psi_{\uparrow B}, \psi_{\downarrow B}, \psi_{\uparrow K}^+, \psi_{\downarrow K}^+, \psi_{\uparrow K^*}^+, \psi_{\downarrow K^*}^+ \}$. Diagonalizing the BdG Hamiltonian, we obtain the energy spectrum. It consists of eight levels with the eigenvalues

$$ E_{0}^{\alpha,\beta} \left( k \right) = \pm \sqrt{\left( \hbar v k \right)^2 + \left( E_0^{\alpha,\beta} \right)^2}, \tag{9.5} $$

with

$$ E_0^{\alpha,\beta} = \sqrt{\left( \lambda_{SO} - \alpha \lambda_V \right)^2 + \Delta_{SC}^2} + \beta \left( \lambda_H + \alpha \lambda_{SX} \right), \tag{9.6} $$

where $\alpha$ and $\beta$ takes $\pm 1$. The gap closes ($E_0^{\alpha,\beta} = 0$) at

$$ \left( \lambda_H + \alpha \lambda_{SX} \right)^2 = \left( \lambda_{SO} - \alpha \lambda_V \right)^2 + \Delta_{SC}^2. \tag{9.7} $$

Though the original Hamiltonian is an $8 \times 8$ matrix, we may decompose it into 4 independent $2 \times 2$ Hamiltonians,

$$ H^{\alpha,\beta} \left( k \right) = \begin{pmatrix} E_0^{\alpha,\beta} & \hbar v k_- - \beta E_0^{\alpha,\beta} \\ -\hbar v k_+ + \beta E_0^{\alpha,\beta} & E_0^{\alpha,\beta} \end{pmatrix}, \tag{9.8} $$

corresponding to $\alpha, \beta = \pm 1$. This Hamiltonian reproduces the energy spectrum ($E_0^{\alpha,\beta}$). We may interpret $\beta E_0^{\alpha,\beta}$ as the modified Dirac mass due to the BCS condensation.

It is straightforward to calculate the Chern number of the superconducting honeycomb system $H_{BdG}$. It is determined by the sign of the modified Dirac mass

$$ C = \frac{1}{2} \sum_{\alpha,\beta = \pm 1} \text{sgn} \left( \beta E_0^{\alpha,\beta} \right). \tag{9.9} $$

The condition of the emergence of a topological superconductivity is $C \neq 0$. Note that it is zero when the time-reversal symmetry is present. In order to obtain a non-zero Chern number, $\lambda_{SX}$ or $\lambda_H$ must be nonzero. It should be noticed that the spin Chern number is no longer defined due to the BCS condensation of the up-spin and down-spin electrons. The topological phase diagram is easily constructed in the $(\lambda_{SO}, \lambda_V, \lambda_{SX}, \lambda_H, \Delta_{SC})$ space. The phase boundaries are given by (9.7). The Chern number is determined from (9.9).

C. Majorana fermion in honeycomb system

We consider a disk region in a honeycomb sheet, as illustrated in Fig[12]. We may tune parameters $\lambda_{SO}$, $\lambda_V$, $\lambda_{SX}$, $\lambda_H$ and $\Delta_{SC}$ to become space-dependent so that the inner region has a different Chern number from the outer region. There appears gapless edge modes at the phase boundary, where $E_0^{\alpha,\beta} \left( r \right) = 0$. According to a general theorem, as we have
reviewed, a zero-energy state with the particle-hole symmetry is always a Majorana fermion.

There are several ways to make $E^{cl}_{\alpha\beta}(r_c) = 0$, since there are four independent mass parameters $\lambda_{SO}$, $\lambda_V$, $\lambda_{SC}$, $\Delta_H$ and one superconducting gap $\Delta_{SC}$. A simple way is to keep only one parameter and $\Delta_{SC}$. We consider the case where electric field is applied to a disk region of an antiferromagnetic topological superconductor ($\lambda_{SC} \neq 0$), as shown in Fig. 12. Very strong electric field can be applied experimentally by an STM probe. We assume electric field is strong enough so that

$$\lambda_V(r) = \ell E_z(r) = \pm \lambda_{SO} + \sqrt{\lambda_{v}^2_{SC} - \Delta_{SC}^2}. \quad (9.10)$$

The critical field is of the order of $E_{c}^{cl} = 0.1 \text{V} \cdot \text{Å}^{-1}$. The inner region of the circle have a nontrivial Chern number $C = 1$ and becomes a topological superconductor. On the other hands, the outer region of the disk have $C = 0$ and remains to be the trivial superconductor. As a result, there emerges one Majorana fermion localized at the boundary of the circle. Its wave function is given by (5.5).

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