Topological Phase Transition and Electrically Tunable Diamagnetism in Silicene

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Silicene has recently been synthesized\cite{1-4} and attracted much attention\cite{5, 2}. It is a monolayer of silicon atoms forming a two-dimensional honeycomb lattice. Almost every striking property of graphene could be transferred to this innovative material. Indeed, its low-energy dynamics is described by the Dirac theory as in graphene. However, Dirac electrons are massive due to a relatively large spin-orbit (SO) gap of 1.55meV in silicene, where the mass can be controlled by applying the electric field $E_z$ perpendicular to the silicene sheet\cite{6}. A novel feature is that silicene is a topological insulator\cite{5}, which is characterized by a full insulating gap in the bulk and helical gapless edges.

Silicene undergoes a topological phase transition from a topological insulator to a band insulator as $|E_z|$ increases and crosses the critical field $E_{cr}$, as has been shown\cite{6} by examining numerically the emergence of the helical zero energy modes in silicene nanoribbons. In this paper we present an analytic result by calculating the topological numbers based on the effective Dirac theory. We show that the origin of the topological numbers is a pseudospin meron in the momentum space. The pseudospin degree of freedom arises from the two-sublattice structure (Fig.1). We also propose a simple method to determine experimentally the phase transition point with the use of the diamagnetism of silicene (Fig.1).

The magnetism of conventional metal is composed of the Pauli paramagnetism due to the spin magnetic moment and the Landau diamagnetism due to the orbital motion of electrons. The free electron system exhibits paramagnetism since the magnitude of the spin component is larger than the orbital component. Contrarily, the Landau diamagnetism overcomes the Pauli paramagnetism in a certain condensed matter system. An extreme case is provided by graphene\cite{8-12}, where the orbital susceptibility has a strong singularity due to the gapless character of Dirac electrons.

We calculate the magnetic susceptibility of silicene as a function of the electric field $E_z$. We expect to have a strong singularity at the critical electric field, $|E_z| = E_{cr}$, since Dirac electrons become gapless at this point\cite{6}. Indeed, we show that it diverges at the critical electric field at zero temperature ($T = 0$), though the divergence is rounded off at finite temperature. However, it is clearly observable as long as $k_B T \lesssim \frac{1}{10} \lambda_{SO}$. Our result is important also from the viewpoint of cross correlation between electric field and magnetism. In general electric-field-controled magnetism is rather difficult compared to magnetic-field-controled electricity. On the other hand, the former is desirable since we can precisely control electric field. Our finding will be important for future electro-magnetic correlated devices.

**TIGHT BINDING MODEL**

Silicene consists of a honeycomb lattice of silicon atoms with two sublattices made of A sites (red) and B sites (blue). The two sublattice planes are separated by a distance. A strong diamagnetism emerges between a magnet and a silicene sheet at the topological phase transition point $E_z = E_{cr}$.

\begin{equation}
H_0 = -t \sum_{\langle i,j \rangle} c_{i\alpha} c_{j\alpha} + i \frac{\lambda_{SO}}{3\sqrt{3}} \sum_{\langle i,j \rangle} \nu_{ij} c_{i\alpha}^\dagger \sigma^z_{\alpha\beta} c_{j\beta} + \frac{2t}{3} \sum_{\langle i,j \rangle} \nu_{ij} c_{i\alpha}^\dagger \left( \sigma \times \hat{d}_{ij} \right)^z_{\alpha\beta} c_{j\beta},
\end{equation}
The band gap $\Delta_0$ as a function of the electric field $E_z$. The gap is open for $E_z \neq \pm E_{cr}$, where silicene is an insulator. It has been shown\cite{18,19} that it is a topological insulator for $|E_z| < E_{cr}$ and a band insulator $|E_z| > E_{cr}$. Thus there occurs a topological phase transition at $|E_z| = E_{cr}$.

The low-energy effective Hamiltonian is derived from the tight binding model

$$H_E = i \lambda_{R1}(E_z) \sum_{\langle i,j \rangle} c_i^\dagger (\sigma \times d_{ij})^z c_j + \ell \sum_{i\alpha} \mu_i E_z c_i^\dagger c_i^\dagger,$$

where $c_i^\dagger$ creates an electron with spin polarization $\alpha$ at site $i$, and $\langle i, j \rangle / \langle i, j \rangle$ 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 coupling with $\lambda_{SO} = 3.9$ meV, where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is the Pauli matrix of spin, with $\nu_{ij} = +1$ if the next-nearest-neighboring hopping is anticlockwise and $\nu_{ij} = -1$ if it is clockwise with respect to the positive $z$ axis. The third term represents the second Rashba SO coupling with $\lambda_{R2} = 0.7$ meV associated with the next-nearest-neighbor hopping term, where $\mu_i = \pm 1$ for the A (B) site, and $d_{ij} = d_{ij} / |d_{ij}|$ with the vector $d_{ij}$ connecting two sites $i$ and $j$ in the same sublattice.

We take a silicene sheet on the $xy$-plane, and apply the electric field $E_z$ perpendicular to the plane. There appear two additional terms in the Hamiltonian,

$$H_E = i \lambda_{R1}(E_z) \sum_{\langle i,j \rangle} c_i^\dagger (\sigma \times d_{ij})^z c_j + \ell \sum_{i\alpha} \mu_i E_z c_i^\dagger c_i^\dagger + \frac{\lambda_{SO}}{\ell} \sum_{i\alpha} c_i^\dagger c_i^\dagger c_i^\dagger c_i\sigma_{\alpha} + \frac{\lambda_{SO}}{2 \ell} \sum_{i\alpha} c_i^\dagger c_i^\dagger c_i^\dagger c_i\sigma_{\alpha},$$

where the first term represents the first Rashba SO coupling associated with the nearest-neighbor hopping, which is induced by external electric field\cite{15,16}. It is proportional to the external electric field, $\lambda_{R1}(E_z) \propto E_z$, and becomes of the order of $10\mu eV$ at $E_z = \lambda_{SO}/\ell = 17$ meVÅ$^{-1}$. The second term is the staggered sublattice potential term $\propto 2\ell E_z$ between silicon atoms at A sites and B sites. The total Hamiltonian is given by $H = H_0 + H_E$. We note that the first Rashba SO coupling term ($\propto \lambda_{R1}$) is missed in the previous analysis\cite{16}.

**DIRAC THEORY**

Electronic states near the Fermi energy are $\pi$ orbitals residing near the K and K' points at opposite corners of the hexagonal Brillouin zone. We also call them the $K_\eta$ points with $\eta = \pm$. The low-energy effective Hamiltonian is derived from the tight binding model $H = H_0 + H_E$. It is described by the

$$H_{\eta} = \hbar v_F (\eta \tau_x \sigma_z + k_\eta \tau_y) + \eta \tau_z h_{11} + \ell E_z \tau_z + \lambda_{R1}(\eta \tau_z \sigma_y - \tau_y \sigma_z)/2,$$

with

$$h_{11} = \lambda_{SO} \sigma_z + a \lambda_{R2} (k_\eta \sigma_x - k_x \sigma_y),$$

where $\tau_z$ is the Pauli matrix of the sublattice pseudospin, $v_F = \sqrt{2} a \ell$ is the Fermi velocity, and $a = 3.86\AA$ is the lattice constant.

The band gap is located at the K and K' points. At these points the energy is exactly given by

$$E_s = \lambda_{SO} + s \ell E_z, \quad \lambda_{SO} + s \sqrt{(\ell E_z)^2 + \lambda_{R1}^2},$$

where $s = \pm 1$ is the spin-chirality. It is given by $s = s_z \eta$ when the spin $s_z$ is a good quantum number. The gap is given by $2|\Delta_+(E_z)|$ with

$$\Delta_+(E_z) = -s \lambda_{SO} + \frac{1}{2} \ell E_z + \frac{1}{2} \sqrt{(\ell E_z)^2 + \lambda_{R1}^2},$$

As $|E_z|$ increases, the gap decreases linearly since $\lambda_{R1} \propto E_z$, and vanishes at the critical point $|E_z| = E_{cr}$ with

$$E_{cr} = \frac{s \lambda_{SO}}{\ell} \left[ 1 - \left( \frac{\lambda_{R1}}{2 \lambda_{SO}} \right)^2 \right] = \pm 17$$.meVÅ,$$

and then increases linearly (Fig 2). The correction due to the first Rashba coupling is extremely small, $(\lambda_{R1}/2\lambda_{SO})^2 = 10^{-4}$.

**SPIN CHERN NUMBER**

We have shown in a previous paper\cite{16} that silicene is a topological insulator for $|E_z| < E_{cr}$ and it is a band insulator for $|E_z| > E_{cr}$ by examining numerically the emergence of the helical zero energy modes in a silicene nanoribbon (Fig 3). In this section we present an analytic discussion by calculating the topological numbers based on the effective Dirac theory.
The topological quantum numbers are the Chern number $C$ and the $\mathbb{Z}_2$ index. If the spin $s_z$ is a good quantum number, the $\mathbb{Z}_2$ index is identical to the spin-Chern number $C_s$ modulo 2. They are defined when the state is gapped, and given by

$$C = C_+ + C_-,$$

$$C_s = \frac{1}{2} (C_+ - C_-),$$

where $C_\pm$ is the summation of the Berry curvature in the momentum space over all occupied states of electrons with $s_z = \pm 1$. They are well defined even if the spin is not a good quantum number.\[17, 18\] A convenient way of calculating the Chern number $C$ and the $\mathbb{Z}_2$ index is to use the formula (6) to the system without the Rashba couplings and then adiabatically switching on these couplings to recover the present system.\[17, 18\]

When we set $\lambda_{R1} = 0$ and $\lambda_{R2} = 0$, the Hamiltonian (3) becomes block diagonal. For each spin $s_z = \pm 1$ and valley $\eta = \pm 1$, it describes a two-band system in the form,

$$H = \tau \cdot \mathbf{d},$$

where

$$d_x = \eta \hbar v_F k_z, \quad d_y = \hbar v_F k_y, \quad d_z = m_D,$$

with the Dirac mass

$$m_D = s \lambda_{SO} + \ell E_z.$$

The summation of the Berry curvature is reduced to the Pontryagin index in the two-band system,\[19\]

$$C^n_{s_z} = \frac{1}{4 \pi} \int d^2 k \left( \frac{\partial \mathbf{d}}{\partial k_x} \times \frac{\partial \mathbf{d}}{\partial k_y} \right) \cdot \mathbf{d},$$

where $\mathbf{d} = \mathbf{d}/|\mathbf{d}|$ is the unit vector which specifies the direction of $\mathbf{d}$. $\mathbf{d}$ is equal to the number of times the unit sphere is covered upon integrating over the Brillouin zone.

It is convenient to use the cylindrical coordinate in the momentum space, where

$$\quad \hat{d}_x \pm i \hat{d}_y = \sqrt{1 - \sigma^2(k)} e^{i \eta \theta}, \quad \hat{d}_z = \sigma(k)$$

with

$$\sigma(k) = \frac{m_D}{\sqrt{(\hbar v_F k)^2 + m_D^2}}$$

The pseudospin texture (13) describes a vortex-like meron in the momentum space, as shown in Fig. 4. The Pontryagin index (12) yields

$$C^n_{s_z} = \frac{\eta}{4 \pi} \int d^2 k \varepsilon_{ij} \partial_i \sigma \partial_j \theta = \frac{\eta}{2} [\Theta / eB] \int_0^{\hat{d}} d\sigma.$$

Hence we find

$$C = \sum_{\eta = \pm} (C^n_{1\eta} + C^n_{2\eta}) = 0,$$

$$C_s = \sum_{\eta = \pm} \frac{1}{2} (C^n_{1\eta} - C^n_{2\eta}) = \Theta (\lambda_{SO} - \ell |E_z|),$$

where $\Theta$ is the step function, i.e.,

$$C_s = \begin{cases} 
1 & \text{for } |E_z| < \lambda_{SO} \\
0 & \text{for } |E_z| > \lambda_{SO}
\end{cases}.$$  

We have verified that the system is a topological insulator for $|E_z| < \lambda_{SO}$ and a band insulator for $|E_z| > \lambda_{SO}$ in the system without the Rashba interactions. The property remains true when they are switched on adiabatically.

**DIAMAGNETISM**

We proceed to discuss a possible experimental method to detect the phase transition point by measuring the magnetic susceptibility. We apply homogeneous magnetic field $\mathbf{B} = \nabla \times \mathbf{A} = (0, 0, -B)$ with $B > 0$ along the z axis to silicene.\[7\] By making the minimal substitution, the Hamiltonian is given by

$$H_B = -\eta (\hbar v_F P_x + P_y) + \eta \tau_z h_{11} + \ell E_z \tau_z + \lambda_{R1} (\eta \tau_z \sigma_y - \tau_y \sigma_z)/2$$

with the covariant momentum $P_i \equiv \hbar k_i + e A_i$. We introduce a pair of Landau-level ladder operators,

$$\hat{a} = \frac{\ell_B (P_x + i P_y)}{\sqrt{2 \hbar}}, \quad \hat{a}^\dagger = \frac{\ell_B (P_x - i P_y)}{\sqrt{2 \hbar}},$$

satisfying $[\hat{a}, \hat{a}^\dagger] = 1$, where $\ell_B = \sqrt{\hbar/eB}$ is the magnetic length. In the basis $\{\psi_{A\uparrow}, \psi_{B\uparrow}, \psi_{A\downarrow}, \psi_{B\downarrow}\}$, the Hamiltonian $H_B$ reads

$$\begin{pmatrix}
\Delta_0^-(E_z) & \hbar \omega_c \hat{a}^\dagger & i \frac{\hbar \omega_c}{\ell_B} \hat{a}^\dagger & 0 \\
\hbar \omega_c \hat{a} & -\Delta_0^-(E_z) & -i \lambda_{R1} & -i \frac{\hbar \omega_c}{\ell_B} \hat{a}^\dagger \\
i \frac{\sqrt{2} \hbar \omega_c}{\ell_B} \hat{a}^\dagger & i \lambda_{R1} & \Delta_0^+(E_z) & \hbar \omega_c \hat{a}^\dagger \\
0 & i \frac{\sqrt{2} \hbar \omega_c}{\ell_B} \hat{a} & \hbar \omega_c \hat{a} & -\Delta_0^+(E_z)
\end{pmatrix}.$$  

(20)
at the K point, with \( \omega_c = \sqrt{2\hbar v_F/\ell_B} \). Here the diagonal elements \( \Delta^0_{\pm} (E_z) \) are

\[
\Delta^0_{\pm} (E_z) = \pm \lambda_{SO} + \epsilon E_z t_z
\]

with the sublattice pseudospin \( t_z \). We note that \( \Delta^\pm (E_z) = \Delta^0_{\pm} (E_z) \) if we set \( \lambda_{RI} = 0 \).

The magnetic susceptibility is defined by

\[
\chi = \frac{M}{B},
\]

where \( M \) is the magnetization and \( B \) is the external magnetic field. The general formula for the orbital magnetic susceptibility of Bloch electrons is given by [20],

\[
\chi = -g_e e^2 \hbar^2 c^2 \sum_n \text{Tr} \left( G v_x G v_y G v_x G v_y \right),
\]

where \( v_i = \partial H/\partial k_i, \beta = 1/k_B T, \) and \( G \) is the temperature Green function

\[
G(k, \omega_n) = (i\hbar\omega_n - H)^{-1},
\]

with \( \hbar\omega_n = (2n + 1) \pi/\beta \) being the Matsubara frequency.

By making the Taylor expansion of (23) with respect to \( \lambda_{RI} \) and \( \lambda_{R2} \), the Rashba terms are found to yield second order corrections, \( \delta\chi = o(\lambda_{RI}^2/\hbar^2 v_F^2) + o(\lambda_{R2}^2/\hbar^2 v_F^2) \), and hence we neglect the Rashba terms in what follows. In this approximation the spin \( s_z \) is a good quantum number.

Integrating out the wave number \( k \) of the matrix trace of (23), we have

\[
\sum_k \text{Tr} \left( G v_x G v_y G v_x G v_y \right) = \sum_{s=\pm} \frac{2}{\hbar^2 \omega_n^2 + \Delta_s^2}.
\]

Using the formula of the infinite sum,

\[
\sum_n \frac{1}{\hbar^2 \omega_n^2 + \Delta_s^2} = \frac{1}{2\Delta_s k_B T} \tanh \frac{\Delta_s}{k_B T},
\]

we obtain the magnetic susceptibility at finite temperature,

\[
\chi(T, E_z) = -g_e e^2 \hbar c^2 \sum_{s=\pm} \frac{1}{\Delta_s} \tanh \frac{\Delta_s}{k_B T}.
\]

where \( g_e = 2 \) represents the valley degree of freedom. We show \( \chi(T, E_z) \) as a function of \( E_z \) for typical values of \( T \).

We can make a precise determination of the critical electric field \( E_{cr} \) based on this formula. Let us consider, for example, a situation where a magnet is placed parallel to a silicene sheet (Fig.1). The magnetization of silicene is given by \( M = -|\chi| B \), where \( B \) is the external magnetic field made by the magnet. The magnet feels a strong repulsive force at \( E_z = E_{cr} \), since we have \( \Delta_s \to 0 \) and \( M \to -\infty \) as \( |E_z| \to E_{cr} \) at \( T = 0 \). Even for finite temperature, \( \chi(T, E_z) \) has a sharp peak at \( |E_z| = E_{cr} \) for \( k_B T \lesssim \lambda_{SO}/10 \) as in Fig.5. Such a strong repulsive force can be detected mechanically.

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