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Topology in single-wall carbon nanotube of zigzag and armchair type

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Abstract. Single-wall carbon nanotubes can be one-dimensional (1D) topological insulators except for armchair nanotubes. The electronic states are characterized by a non-zero topological invariant, winding number, which is related to the number of 0D edge states via the bulk-edge correspondence. In the present study, we theoretically examine zigzag and armchair nanotubes to elucidate the emergence and absence of edge states. The effective 1D lattice model is employed in order to describe the fine structures due to the finite curvature of tube surface and spin-orbit interaction. We show that the lattice model for a zigzag nanotube is equivalent to the Su-Schrieffer-Heeger model, by which the formation of edge states is explained. An armchair nanotube is described by a ladder model, on the other hand, which does not host any edge states owing to the σₕ symmetry.

1. Introduction
The single-wall carbon nanotube (SWNT) is a unique one-dimensional (1D) system made by rolling up a graphene sheet. It can be either metallic or semiconducting depending on its chirality [1]. Even for a metallic SWNT, a narrow energy gap opens between conduction and valence bands due to the mixing of σ and π orbitals by the finite curvature of tube surface [2, 3] and spin-orbit (SO) interaction [4].

Both metallic and semiconducting SWNTs can be regarded as 1D topological insulators owing to the sublattice symmetry for A and B lattice sites. The electronic states are characterized by a Z topological invariant, winding number [5], in both the absence (class BDI) and presence (AIII) of magnetic field [6]. The winding number is related to the number of 0D edge states in finite SWNTs with a suitable boundary condition via the bulk-edge correspondence [7]. The present authors revealed that SWNTs except for armchair nanotubes may be topologically non-trivial in general [8]. Besides, in metallic SWNTs, the small band gap is closed by applying a feasible magnetic field B in the axial direction, which results in the topological phase transition. This phase transition should be observed as a change in the number of edge states, e.g., using scanning tunneling spectroscopy [9].

In this work, we elucidate the mechanism of emergence and absence of the edge states in SWNTs. For this purpose, we examine a 1D lattice model proposed in Ref. [8], which effectively describes the curvature effects and SO interaction. As an example of non-trivial topological
Figure 1. (a) Primitive lattice vectors of graphene, $a_1$ and $a_2$, and mapping of $(n, m)$-SWNT to the graphene sheet [8]. The chiral vector, $C_h = na_1 + ma_2$, indicates the circumference of the tube. The three vectors $\Delta^{(1)}_j$ ($j = 1, 2, 3$) connect the nearest-neighbor atoms, whereas the six vectors $\Delta^{(2)}_j$ ($j = 1, 2, \ldots, 6$) connect the second nearest-neighbor atoms. The rotational symmetry $C_d$ around the tube axis (helical symmetry) corresponds to the translational symmetry of $C_h/d$ ($R = pa_1 + qa_2$), where $d = \text{gcd}(n, m)$, and $p$ and $q$ are integers satisfying $mp - nq = d$. This figure shows the case of $(n, m) = (6, 3)$ with $d = 3$, $p = 1$, and $q = 0$. (b) An effective 1D lattice model in which $A$ and $B$ atoms are aligned in the axial direction. The distant hoppings $\Delta^\ell_{ij}$ and phase factor $\Delta^\nu_{ij}$ of $H$'s in Eq. (1) are determined from $\Delta^{(i)}_j = \Delta^\ell_{ij}R + \Delta^\nu_{ij}(C_h/d)$ [12].

To understand the electronic properties of SWNTs, a zigzag nanotube is studied. Its lattice model is shown to be equivalent to the Su-Schrieffer-Heeger (SSH) model, which is known as a fundamental model for 1D topological insulators [10]. The formation of edge states and topological phase transition are clearly explained in terms of the SSH model. For an armchair nanotube, on the other hand, the winding number is always zero and thus it is topologically trivial. Its lattice model is mapped to a ladder model, which is extended from that in Ref. [11] to take into account the SO interaction as well as axial symmetry. We show that it does not host any edge states due to the $\sigma_h$ symmetry [7].

2. Model
We consider a SWNT whose circumference is specified by the chiral vector, $C_h = na_1 + ma_2 \equiv (n, m)$, with $a_1$ and $a_2$ being the primitive lattice vectors of graphene shown in Fig. 1 (a) [1]. For zigzag and armchair nanotubes, we use $(n, 0)$- and $(n, n)$-SWNTs with $n > 0$, respectively. The diameter is given by $d = |C_h|/\pi = a\sqrt{n^2 + nm + m^2}/\pi$ with the lattice constant $a = 0.246$ nm of graphene. The chiral angle $\theta$ is defined as the angle between $C_h$ and $a_1$: $\theta = 0$ and $\pi/6$ for zigzag and armchair types, respectively.

$(n, m)$-SWNT has the $d$-fold symmetry around the tube axis, where $d = \text{gcd}(n, m)$ is the greatest common divisor of $n$ and $m$. It also has the helical symmetry with translation along the tube axis with a rotation around it [13]. Due to these symmetries, the electronic states in $(n, m)$-SWNT with orbital angular momentum $\mu = 0, 1, 2, \ldots, d - 1$ is described by a 1D lattice model shown in Fig. 1 (b). Starting from the $\mathbf{k} \cdot \mathbf{p}$ theory to consider the curvature effects and SO interaction [14], we construct a 1D lattice model to describe the electronic states around the $K$ and $K'$ points [8].
is given by

\[ H_{\mu,s} = \sum_{\sigma,\ell} \frac{1}{2} g_\sigma \mu_B B s c_{\sigma,\ell}^{\mu,s} \{ (\gamma_{s,j}^{(1)}) e^{i(1)\phi_j} c_{A,\ell}^{\mu,s} c_{B,\ell}^{\mu,s} + h.c. \} \]

\[ + \sum_{\sigma,\ell} \sum_{j=1}^{3} (\gamma_{s,j}^{(2)}) e^{i(2)\phi_j} c_{\sigma,\ell}^{\mu,s} c_{\sigma,\ell}^{\mu,s} + h.c. ) \].

(1)

Here, \( c_{\sigma,\ell}^{\mu,s} \) is the field operator of an electron with angular momentum \( \mu \) and spin \( s \) at atom \( \sigma = A, B \) of site index \( \ell \). The hopping to the first [second] nearest-neighbor atoms in Fig. 1 (a) gives rise to the hopping to the site separated by \( \Delta \ell \) \([\Delta \ell] \) with phase factor \( \Delta \phi \) \([\Delta \phi] \), as depicted in Fig. 1 (b). The hopping integrals \( \gamma_{s,j}^{(1)} \) and \( \gamma_{s,j}^{(2)} \) are given by

\[ \gamma_{s,j}^{(1)} = \gamma [1 + \Delta k_{s0} c_{s}\sin \phi_j - i(\Delta k_s + i(\Delta k_{s0} + \Delta k_{s})) a_{CC} \cos \phi_j] \}, \]

\[ \gamma_{s,j}^{(2)} = i(-1)^j+1 \frac{3}{2V} \sin \phi_j \]

respectively, where \( \phi_j = \theta - (5\pi/6) + (2\pi/3)j \), \( a_{CC} = a/\sqrt{3} \) is the interatomic distance, and \( \gamma = -2\hbar v_F/(3a_{CC}) \) with \( v_F = 8.32 \times 10^6 \) m/s being the Fermi velocity. The hybridization between \( \sigma \) and \( \pi \) orbitals due to the finite curvature is taking into account by

\[ \Delta k_\ell = \beta' \cos 3\theta \frac{\sin \phi_j}{d_\ell^2}, \quad \Delta k_z = \zeta \frac{\sin 3\theta}{d_\ell^2}, \]

(4)

with \( \beta' = 0.0436 \) nm and \( \zeta = -0.185 \) nm. The SO interaction yields

\[ \Delta k_{s0} = \alpha' V_{so} \frac{1}{d_\ell^2}, \quad \epsilon_{s0} = \alpha_2 V_{so} \frac{\cos \theta}{d_\ell}, \]

(5)

with \( \alpha' = 8.8 \times 10^{-5} \) meV\(^{-1}\), \( \alpha_2 = -0.045 \) nm, and \( V_{so} = 6 \) meV being the SO interaction for 2p orbital in carbon atom. The Aharonov-Bohm (AB) phase by magnetic field \( B \) appears as

\[ \Delta k_\phi = -\frac{eB}{4\hbar} d_\ell. \]

(6)

For a metallic SWNT, the local gap in the vicinity of \( K/K' \) points yields

\[ E_g = 2\hbar v_F |\pm \Delta k_c + s\Delta k_{s0} + \Delta k_\phi|, \]

(7)

for electrons with spin \( s \).

3. Zigzag nanotube

We consider \((n,0)\)-SWNT as a zigzag nanotube with \( n > 0 \). It is semiconducting when \( n \neq 0 \) (mod 3) and metallic when \( n = 0 \) (mod 3). For a semiconducting nanotube, the band gap is given by the boundary condition in the circumference direction, and the fine structures are irrelevant. For a metallic nanotube, the band gap is dominantly determined by \( \Delta k_c \), whereas the SO interaction brings about small corrections. We therefore neglect the SO interaction as well as Zeeman energy for a while. The effective 1D lattice model in Eq. (1) is reduced to [15],

\[ H_{\mu,s} = \sum_\ell \left( \gamma_{\text{intra}}^{\mu,s} c_{A,\ell}^{\mu,s} c_{B,\ell}^{\mu,s} + \gamma_{\text{inter}}^{\mu,s} c_{A,\ell}^{\mu,s} c_{B,\ell+1}^{\mu,s} \right) + h.c., \]

(8)
Figure 2. (a) The effective 1D lattice model for a zigzag nanotube. The SO interaction is neglected. This is equivalent to the SSH model with staggered hopping integrals, determined by $\mu$, $d_t$, and $B$. (b) When the hopping amplitude within the unit cell is weaker than that between the adjacent cells, $|\gamma^{\mu,s}_{\text{intra}}| < |\gamma^{\mu,s}_{\text{inter}}|$, the model is topologically equivalent to the inter-cell dimerization with 0D edge states. (c) On the other hand, for $|\gamma^{\mu,s}_{\text{inter}}| > |\gamma^{\mu,s}_{\text{intra}}|$, the system hosts no edge states.

with

$$
\gamma^{\mu,s}_{\text{intra}} = 2\gamma e^{-\frac{\pi n}{2}} \left[ e^{\Delta k_c a_{CC}} \cos \left( \frac{\pi \mu}{n} - \frac{3}{2} \Delta k_\phi a_{CC} \right) \right], \quad \gamma^{\mu,s}_{\text{inter}} = \gamma e^{\Delta k_c a_{CC}}.
$$

This model, as shown in Fig. 2 (a), is equivalent to the SSH model for polyacetylene, which is a well known 1D topological insulator [10]. The topological nature of SSH model is classified by the ratio of the hopping amplitude within the unit cell to that between adjacent cells,

$$
\alpha = \left| \frac{\gamma^{\mu,s}_{\text{intra}}}{\gamma^{\mu,s}_{\text{inter}}} \right| = 2 e^{-\frac{3}{2} \Delta k_c a_{CC}} \left| \cos \left( \frac{\pi \mu}{n} - \frac{3}{2} \Delta k_\phi a_{CC} \right) \right|.
$$

For angular momenta at the $K/K'$ points ($\mu K/K' = \pm 2n/3$), we have

$$
\alpha = e^{-\frac{3}{2} (\Delta k_c \pm \Delta k_\phi) a_{CC}}.
$$

When $\alpha = 1$, the gap is closed and the winding number cannot be defined. For $\alpha < 1$, the system can be adiabatically deformed into that with $\gamma_{\text{intra}} = 0$, as shown in Fig. 2 (b). The system has 0D edge states at zero energy. At the same time, the winding number becomes finite, and the system is topologically non-trivial. On the other hand, for $\alpha > 1$, the system can be deformed into that with $\gamma_{\text{inter}} = 0$, as depicted in Fig. 2 (c), which has no edge states at zero energy. As a result, the winding number becomes zero, and the system is a trivial insulator.

By counting the angular momenta $\mu$ that satisfy $\alpha < 1$, we find that the number of edge states is

$$
4[(n/3) + 1] \text{ for } n = 0 \text{ (mod 3)},
$$

$$
4[(n/3) + \text{mod}(n, 3) - 1] \text{ for } n \neq 0 \text{ (mod 3)},
$$

at $B = 0$ with $[x]$ being the greatest integer not exceeding $x$. Consequently, a zigzag nanotube is shown to be a topological insulator at $B = 0$.

Equation (11) clearly explains the topological phase transition in a metallic zigzag nanotube, where the local gap around the $K$ point disappears for $B = B^*$ at which $\Delta k_c + \Delta k_\phi = 0$ is satisfied. When $B < B^*$, $\alpha < 1$ for $\mu = \mu K$, and the system hosts edge states from the $K$ valleys. When $B > B^*$, $\alpha > 1$ for $\mu = \mu K$, and the edge states from the $K$ valley are delocalized. This is the topological phase transition discussed in Ref. [8]. Note that a similar phase transition takes place at $B = -B^*$ for the $K'$ valley.

We also consider the effects of the SO interaction and Zeeman energy. Our numerical calculation shows that edge states in typical zigzag nanotubes with $d_t \sim 1$ nm can well be explained by the above-mentioned scenario.
Figure 3. (a) The effective 1D lattice model for an armchair nanotube. Note that $|\gamma^\mu s_+| = |\gamma^\mu s_-|$ owing to the $\sigma_h$ symmetry. (b) The equivalent ladder model after swapping $A$ and $B$ atoms at even sites.

4. Armchair nanotube

Next, we consider $(n, n)$-SWNT as an armchair nanotube with $n > 0$. It is always metallic independent of $n$. Since $\Delta k_c = 0$, the small energy gap is determined by $\Delta k_{so}$. Neglecting the small Zeeman splitting, the corresponding 1D lattice model yields [16],

$$H_{\mu,s} = \sum_\ell \left( \gamma^\mu s_0 c^\mu_A,\ell c^\mu_B,\ell \gamma^\mu s_+ c^\mu_A,\ell c^\mu_B,\ell+1 \gamma^\mu s_- c^\mu_A,\ell c^\mu_B,\ell-1 \right) + \text{h.c.},$$

with

$$\gamma^\mu s_0 = \gamma e^{-i[(\Delta k_\varphi + s\Delta k_{so}) + \Delta k_\delta]a_{CC}}, \quad e^{i2\pi\mu/\ell}\gamma^\mu s_+ = \gamma e^{i[(\Delta k_\varphi + s\Delta k_{so}) + \Delta k_\delta]a_{CC}},$$

as shown in Fig. 3 (a). Note that $|\gamma^\mu s_+| = |\gamma^\mu s_-|$ due to the mirror reflection, $\sigma_h$, symmetry with a horizontal mirror plane perpendicular to the nanotube axis. This model is depicted in Fig. 3 (b), if $A$ and $B$ sublattices are exchanged in a similar manner to Ref. [11]. The gap disappears at a magnetic field which satisfies $\Delta k_\varphi + s\Delta k_{so} = 0$ with $s = +1$ or $-1$. Otherwise, the system becomes an insulator, on which we focus hereafter. We find that, unlike the case of a zigzag nanotube, there cannot be any edge state; the system can be adiabatically deformed into that with $|\gamma^\mu s_+| = |\gamma^\mu s_-| = 0$, which is the same situation as shown in Fig. 2 (c). This fact clearly explains that an armchair nanotube cannot host edge states for any $\mu$ and $s$ and thus it is a trivial insulator. Note that the Zeeman splitting is irrelevant also in the case of an armchair nanotube.

5. Conclusions

We have theoretically examined the properties of zigzag and armchair SWNTs as topological insulators, by observing edge states in an effective 1D lattice model to take into account the finite curvature and SO interaction. The lattice model for a zigzag nanotube is equivalent to the SSH model, by which the emergence of edge states as well as magnetic-field-induced topological phase transition have been clearly explained. The lattice model for an armchair nanotube is a ladder model, on the other hand, which does not host any edge states owing to the $\sigma_h$ symmetry.

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[16] We choose $(p, q) = (1, 0)$ to minimize $|R|$. 