Edge state in AB-stacked bilayer graphene and its correspondence with SSH ladder

Tixuan Tan,1,2† Ci Li,1,2† and Wang Yao1,2

1Department of Physics, The University of Hong Kong, Hong Kong, China
2HKU-UCAS Joint Institute of Theoretical and Computational Physics at Hong Kong, China

We study edge states in AB-stacked bilayer graphene (BLG) ribbon where the Chern number of the corresponding two-dimensional (2D) bulk Hamiltonian is zero. The existence and topological features of edge states when two layers ended with the same or different edge terminations (zigzag, bearded, armchair) are discussed. The edge states (non-dispersive bands near the Fermi level) are states localized at the edge of graphene nanoribbon that only exists in a certain range of momentum \( k_y \). Their existence near the Fermi level are protected by the chiral symmetry with topology well described by coupled Su-Schrieffer-Heeger (SSH) chains model, i.e., SSH ladder, based on the bulk-edge correspondence of one-dimensional (1D) systems. These zero-energy edge states can exist in the whole \( k_y \) region when two layers have zigzag and bearded edges, respectively. Winding number calculation shows a topological phase transition between two distinct non-trivial topological phases when crossing the Dirac points. Interestingly, we find the stacking configuration of BLG ribbon is important since they can lead to unexpected edge states without protection from the chiral symmetry both near the Fermi level in armchair-armchair case and in the gap within bulk bands that are away from Fermi level in the general case. The influence of interlayer next nearest neighbor (NNN) interaction and interlayer bias are also discussed to fit the realistic graphene materials, which suggest the robust topological features of edge states in BLG systems.

I. INTRODUCTION

One of the most attractive phenomena in condensed matter physics is the existence and behavior of edge states, whose wave function is localized at the system’s edge, of two-dimensional (2D) systems. These states are different from the bulk states in properties and play important roles in transport, e.g., quantum Hall effect (QHE) and the quantum spin Hall effect (QSHE). On the other hand, the existence and properties of zero-energy edge states near the Fermi level (flat bands) are usually connected with the non-trivial topological phases of the bulk system by the bulk-edge correspondence, which can be distinguished by the specific symmetry of the system and topological invariants such as the winding number.

After the progress in a decade, graphene, or the nanotube and nanoribbon, has become one of the most active two-dimensional nanomaterial in condensed matter physics due to excellent electrical and mechanical properties. The free standing monolayer graphene (MLG) is a zero-gap semiconductor where the conduction and valance band touch each other at the Dirac point. It has a trivial bulk topology as two inequivalent valleys provide opposite topological charges, leading to a zero Chern number. However, edge states still exist in such graphene systems as non-dispersive bands (flat bands) at the Fermi level, which are observed by supposing a semi-infinite system, with quantized wave vectors \( k_y \) in the infinite direction. The existence of these non-dispersive edge states and related topology in the MLG can be further described by the bulk-edge correspondence between the winding number or Zak phase of one-dimensional (1D) SSH chain systems and the existence of a localized state at the chain’s edge, as shown in Fig. 1.

On the other hand, due to the equivalence between the graphene system and the honeycomb bosonic lattice system, i.e., the 2D magnon system which generally results from the collinear Ferromagnet after Holstein-Primakoff transformation, edge states similar to those observed in MLG can also be found in both the related honeycomb bosonic lattice and even non-honeycomb bosonic lattice. There are also both experimental and theoretical study on other types of edges states in photonic honeycomb lattice using different models.

In this article, we focus on the existence and topology of edge states in AB-stacked bilayer graphene (BLG) ribbon by connecting them with \( k_y \)-parameterized SSH ladder. Earlier works are mainly concentrated on the existence of edge states of BLG under specific edge conditions and related equivalent bilayer magnon systems or the behavior of edge states when various symmetry-breaking terms are added. Here the AB-stacked BLG ribbon we discuss involves three conventional edges (zigzag, bearded, and armchair, as shown in Fig. 1), whose bulk 2D system always has zero Chern number. Interlayer next nearest neighbor (NNN) interaction and interlayer bias are considered in terms of their influence on the topology of SSH ladder. A detailed topological classification based on discrete symmetry and topological invariants calculation for effective 1D bulk Hamiltonian of SSH ladder \( H(k_y, k) \) parameterized by \( k_y \) of AB-stacked BLG ribbon with various types of edge are performed, as shown in Table 1. It shows the zero-energy edge states can only exist when chiral symmetry is preserved for \( k_y \) and can appear in the whole \( k_y \) region when two layers of BLG ribbon have zigzag and bearded edge, respectively. On the other hand, straightforward calculation shows that unexpected edge states can exist in the gap within bulk bands that are away from the Fermi level. These edge states are unprotected...
by the chiral symmetry and are dependent on the specific edge configurations of BLG ribbon. Interlayer bias is included in our discussion as it explicitly breaks the chiral symmetry responsible for the existence of zero-energy edge states. However, edge states still exist after this chiral symmetry breaking as non-zero energy states.

The rest of paper is organized as follows. We first give a brief review on the existence of edge states and topology of MLG ribbon in Sec. II as a basis for our discussion of AB-stacked BLG ribbon. In Sec. III we turn to the behavior and topology of edge states in AB-stacked BLG ribbon and their correspondence with SSH ladder $H(k_y,k)$. Then we discuss the geometrical origin of the edge states appearing in the gap within bulk bands that are away from the Fermi level in Sec. IV. Finally, we present our conclusions in Sec. V as a summary.

II. EDGE STATES IN THE MLG RIBBON

To discuss the existence and topological features of edge states in AB-stacked BLG ribbon, we first give a brief review of the edge states in the MLG ribbon. In general, MLG tight-binding Hamiltonian with nearest neighbor (NN) hopping energy $t$ and on-site potential $U_i$ can be written as

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + \sum_i U_i c_i^\dagger c_i,$$  

where $\sum_{\langle i,j \rangle}$ sums over only NN pairs. The lattice primitive vectors are $\vec{a}_1$ and $\vec{a}_2$, which are shown in Fig. 1. As examples and without loss of generality, we mainly consider nanoribbons with three different types of edges: zigzag, bearded, and armchair in $y$ direction and enforce the periodic boundary condition (PBC) along this direction to see the edge states, as shown in Fig. 1(a), (b), and (c), respectively.

A. MLG with bearded (zigzag) edges

The tight-binding Hamiltonian of a MLG with a bearded edge in $y$ direction, as shown in Fig. 1(a), can be expressed as

$$H_{\text{bea}} = -t \sum_{m=1}^{M} \sum_{n=1}^{N} \left\{ a_{m,n}^\dagger b_{m,n} + b_{m,n}^\dagger \left( a_{m,n+1} + a_{m+1,n+1} \right) \right\}$$

$$-b_{m,N}^\dagger \left( a_{m,1} + a_{m+1,1} \right) + \text{H.c.},$$

where $a_{m,n}$ ($a_{m,n}^\dagger$) annihilates (creates) an electron on site $(m,n)$ on sublattice $A$ (an equivalent definition is used for sublattice $B$). The system is assumed infinite along $m$ direction and finite along $n$ direction. The minus term in the curly brackets gives the open boundary condition (OBC) in the finite direction. The Fourier transformation along the infinite direction is

$$f_{m,n} = \frac{1}{\sqrt{M}} \sum_{k_y} e^{ik_y m} f_{k_y,n}, f = a,b,$$

$$k_y = \frac{2\pi (m - M/2)}{M}, m = 0,1,2,\ldots,M-1,$$

and leads to

$$H_{\text{bea}}(k_y) = -t \sum_{n=1}^{N-1} \left\{ a_{k_y,n}^\dagger b_{k_y,n} + (1 + e^{ik_y}) b_{k_y,n}^\dagger a_{k_y,n+1} \right\}$$

$$+ a_{k_y,N}^\dagger b_{k_y,N} + \text{H.c.},$$

which is equivalent to an effective SSH chain parameterized by $k_y$ as below. Notice that we have made a redefinition of basis by a phase such that the hopping becomes real and it is easier to make association with the original SSH chain model. Not doing such a redefinition would leave the coupling complex, but all results in this paper are not affected.

$$H_{\text{bea}}(k_y) \simeq \sum_{n=1}^{N-1} \left( v a_{n}^\dagger b_n + w b_{n}^\dagger a_{n+1} \right) + v a_{N}^\dagger b_N + \text{H.c.},$$

$$w = -2t \cos \frac{k_y}{2}, v = -t.$$

The bulk Hamiltonian of this equivalent chain is

$$H_{\text{bea}}(k_y,k) = \eta h_b(k_y,k),$$

$$h_b(k_y,k) = \begin{bmatrix} 0 & v + w e^{ik} \\ v + w e^{-ik} & 0 \end{bmatrix},$$

which belongs to the non-trivial topological class $BDL$ (see Table I for details).

We plot the band structure of bearded-edge graphene nanoribbon and winding number for the bulk Hamiltonian $H_{\text{bea}}(k_y,k)$ [6] as a function of parameter $k_y$ in Fig. 2(a), respectively. The winding number we used in this paper is defined as

$$W = -\frac{i}{4\pi} \int_{BZ} \text{d}k \text{Tr} (SQ^{-1} \partial_k Q),$$

where

$$S = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$$

and

$$Q = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}.$$
with

\[ Q(k) = I_N - 2\mathcal{P}(k), \mathcal{P}(k) = \sum_{\alpha < 0} |u_\alpha\rangle \langle u_\alpha|, \quad (8) \]

\( \alpha < 0 \) refers to the occupied bands (eigenstates of \( H(k_y, k) \) below the Fermi level). \( Q^{-1}(k) = Q(k) \), as \( Q^2 = I_N \). Winding number describes the topological properties near the zero energy (Fermi level) of 1D bulk Hamiltonians \( H(k_y, k) \) with the chiral symmetry operator \( S \). Here we would like to stress again one should not confuse \( k_x \) with \( k_y \) since \( k_y \) appearing in the bulk Hamiltonian \( H(k_y, k) \) is a parameter of the system and \( k \) is the wave vector of the effective SSH chain when its length is taken to be infinite. The integration appearing in the definition of \( W \) is over \( k \), with \( W \) being a function of \( k_y \). A concrete example with some details omitted here is given in the Appendix to make clear the origin of \( k_y \) and \( k \).

The zero-energy edge states (flat bands) exist in the restricted region \( k_y \in [-\pi, -\frac{2\pi}{3}] \cup \left\{ \frac{2\pi}{3}, \pi \right\} \) and correspond \( W = 1 \), which agree with previous literature.\(^\text{27,11}\) The effective 1D Hamiltonian \( H_{\text{sig}}(k_y) \) for a MLG with a zigzag edge can be obtained by switching \( w \) and \( v \), \( a_n \) and \( b_n \) in \( H_{\text{bea}}(k_y) \) as zigzag edge is related with bearded edge through an exchange of basis and coupling (see Fig. 1(a) and (b)). In terms of their corresponding SSH chain, zigzag nanoribbon and bearded nanoribbon differ from each other by a switch between intercell coupling and intracell coupling of the chain. It can be observed from Fig. 2(a) and (b) that zero-energy edge states (flat bands) of \( H_{\text{sig}}(k_y) \) and non-zero winding number of \( H_{\text{sig}}(k_y, k) \) appear in complementary region of \( k_y \) to the one with bearded edges.

**B. MLG with armchair edges**

The tight-binding Hamiltonian of a MLG ribbon with an armchair edge is different from the previous case, which is

\[ H_{\text{arm}} = -t \sum_{n=1}^{M/2} \sum_{m=1}^{N} (a_{2m,n}^\dagger b_{2m,n} + b_{2m,n}^\dagger a_{2m,n+1}) + a_{2m-1,n}^\dagger b_{2m-1,n} + b_{2m-1,n}^\dagger a_{2m-1,n} + \sum_{m=1}^{M} a_{m+1,n}^\dagger b_{m,n} + \sum_{m=1}^{M/2} \left( b_{2m,N}^\dagger a_{2m,1} + b_{2m-1,1}^\dagger a_{2m-1,N} \right) + \text{H.c.}, \quad (9) \]

where \( M/2 \in \mathbb{N} \). Unit with translational symmetry of this ribbon in Fig. 1(c) is constructed as \( (m, n) \approx (b_{2m-1,n}, a_{2m-1,n}, a_{2m,n}, a_{2m,n+1}) \). The effective Hamiltonian parameterized by \( k_y \) for this ribbon is no longer a single SSH chain but two coupled uniform chains as shown in Fig. 1(c). The coupled chains have the bulk Hamiltonian:

\[ H_{\text{arm}}(k_y, k) = \eta |h_{a}(k_y, k)\rangle \langle h_{a}(k_y, k)| = (b_k^a, a_k^a, a_k^a)\),
\[ h_{a}(k_y, k) = -t \begin{bmatrix} h(k) & D(k_y) & h(k) \\ \end{bmatrix}, \quad (10) \]

\[ D(k_y) = \begin{bmatrix} 0 & 1 + e^{-ik} \\ 1 + e^{ik} & 0 \end{bmatrix}, \quad (11) \]

where the superscript 1/2 distinguishes even and odd since there are two sets of A/B in each unit of armchair MLG shown in Fig. 1(c):

\[ f_{k}^1 = \frac{1}{\sqrt{N}} \sum_{j=1}^{M/2} \sum_{n=1}^{N} \sum_{j=1}^{M/2} \sum_{n=1}^{N} e^{-ikn} e^{-ikyj} f_{2j-1,n} \]
\[ f_{k}^2 = \frac{1}{\sqrt{N}} \sum_{j=1}^{M/2} \sum_{n=1}^{N} \sum_{j=1}^{M/2} \sum_{n=1}^{N} e^{-ikn} e^{-ikyj} f_{2j,n} \]

\( f = a, b \) as shown in Fig. 1. Notice, again, \( k \) is the wave vector of the coupled chains while \( k_y \) is a parameter of its coupling. This bulk Hamiltonian of the coupled chains belongs to the non-trivial topological class \( AIII \) (see Table 1 for detail). Here we would like to point out that although it belongs to the non-trivial topological class, the winding number is zero in the whole region of \( k_y \) and there are no edge states, as shown in Fig. 2(c), which means this is a trivial case.

**III. EDGE STATES NEAR THE ZERO ENERGY (FERMI LEVEL) IN THE AB-STACKED BLG**

Based on the three different graphene nanoribbons discussed in last section, there are four types of AB-stacke
TABLE I. Topological classification for different effective 1D bulk Hamiltonians $H(k_y, k)$ of SSH chain/ladder. The related winding number $W$ and number of zero-energy edge states $N_{ES}$ are also shown. The topological classification is based on the the presence or absence (0) of time-reversal ($T$), particle-hole ($C$), and chiral ($S$) symmetries $^{[70]}$ where all three symmetry operators are unitary, i.e., $O^T O = 1 = T, C, S$. They satisfy $T^* H^*(k_y, k) T = H(k_y, -k), C^* H^*(k_y, k) C = -H(k_y, -k), S^* H(k_y, k) S = -H(k_y, k)$, respectively. $\pm$ in $T$ and $C$ comes from $T^* T = \pm 1$ and $C^* C = \pm 1$. $I_N$ is $N \times N$ identity matrix. \(\sigma_z\) represent Pauli matrices. \(\alpha\) means that there is no well-defined winding number since the chiral symmetry is broken. $^{[83]}$ Notice that when operator is written in direct product form, they can be understood as acting on different degrees of freedom (DOF). For example, $S = I_2 \otimes \sigma_z$ for $H_{\text{bea-bea}}$, where $I_2$ acts on layer DOF and $\sigma_z$ acts on sublattice DOF.

| Effective 1D bulk Hamiltonian | $T$ | $C$ | $S$ | Class | $W$ | $N_{ES}$ |
|-------------------------------|-----|-----|-----|-------|-----|--------|
| $H_{\text{bea\_zig}}(k_y, k)$ (Eq. 6) | $I_2(\pm)$ | $\sigma_z(\pm)$ | $\sigma_z$ | BDI | 1, 0 (Fig. 2) | 2 (Fig. 2) |
| $H_{\text{arm\_arm}}(k_y, k)$ (Eq. 10) | 0 | 0 | $\sigma_z \otimes \sigma_z$ | AIII | 0 (Fig. 2) | 0 (Fig. 2) |
| $H^\dagger_{\text{arm\_arm}}(k_y, k)$, $U = 0$ (Eq. 14) | 0 | 0 | $I_2 \otimes \sigma_z \otimes \sigma_z$ | AIII | 0 | 0 (Fig. 4) |
| $H_{\text{arm\_arm}}(k_y, k)$, $U = 0$ (Eq. 14) | 0 | 0 | $I_2 \otimes \sigma_z \otimes \sigma_z$ | AIII | 0 | 0 (Fig. 4) |
| $H^\dagger_{\text{bea\_bea\_zig\_zig}}(k_y, k)$, $U = 0$ (Eq. 16) | $I_2(\pm)$ | $I_2 \otimes \sigma_z(\pm)$ | $I_2 \otimes \sigma_z$ | BDI | 2, 0 (Fig. 7) | 4 (Fig. 7) |
| $H_{\text{bea\_bea\_zig\_zig}}(k_y, k)$, $U \neq 0$ (Eq. 16) | $I_2(\pm)$ | 0 | $I_2 \otimes \sigma_z(\pm)$ | BDI | 2, 0 (Fig. 7) | 4 (Fig. 7) |
| $H^\dagger_{\text{bea\_bea\_zig\_zig}}(k_y, k)$, $U = 0$ (Eq. 19) | $I_2(\pm)$ | $\sigma_z \otimes \sigma_z(\pm)$ | $\sigma_z \otimes \sigma_z$ | BDI | -1, 1 (Fig. 7) | 2 (Fig. 7) |
| $H_{\text{bea\_bea\_zig\_zig}}(k_y, k)$, $U \neq 0$ (Eq. 19) | $I_2(\pm)$ | 0 | $\sigma_z \otimes \sigma_z(\pm)$ | BDI | -1, 1 (Fig. 7) | 2 (Fig. 7) |

FIG. 3. (Color online) The atomic structure of AB-stacked BLG in side view.

BLG ribbon, i.e., arm-arm (both layers are armchair edges), zig-zig/bea-bea (both layers are zigzag or bearded edges), bea-zig (one layer is bearded edges and the other is zigzag edges), as listed in Table. I. They can be summarized by the tight-binding Hamiltonian $^{[19][52]}$

$$H = \sum_{l} H^l_{\text{edge}} + H_{\text{int}} + H_{\text{on-site}},$$

(12)

where $l = 1, 2$ are labels of the bottom and top layers respectively. $H_{\text{on-site}}$ refers to the on-site energy of carbon atoms such as interlayer bias $U$ as shown in Fig. 3. It includes contribution from both layers. $H_{\text{int}}$ describes the van der Waals interaction between two layers. $^{[19][52]}$ The meanings of various interlayer couplings $\gamma_i$ with $i = 1, 3, 4$ are indicated in Fig. 2. Here, we take $t = 3.16eV, \gamma_1 = 0.381eV$ as typical experimental values for AB-stacked BLGs $^{[53]}$ and $\gamma_4 = 0$ throughout this work since it is pretty small compared with others in realistic systems $^{[17][19][53]}$. We choose $\gamma_3 = 0.38eV \approx \gamma_1$ when considering the non-zero $\gamma_3$, which is close to most of the experimental observations $^{[19][12][53]}$.

A. AB-stacked BLG with armchair-armchair edges

Next we will discuss these four types of AB-stacked BLG structures in detail. To form an AB-stacked BLG ribbon, armchair MLG can only be stacked with the other armchair MLG, but not with zigzag/bearded MLG (see
Fig. 5. (Color online) Right panel: The atomic structure of an armchair-armchair AB-stacked BLG ribbon in top view, corresponding to 1D effective Hamiltonian $H_{\text{arm-arm}}(k_y, k)$ (Eq. 14). The edge configuration is parameterized by $y = \frac{1}{e} V$. The red solid lines are the edge states. There are four of them. The wave function distribution in real space of a typical edge state in red dashed box is shown on the right side. Vertical axis is wave function amplitude, and the horizontal axis is the site index, which increases along the finite direction of the ribbon.

Thus, we first consider the Hamiltonian

$$H_{\text{arm-arm}} = \sum_i H_{\text{arm}}^i + H_{\text{int}} + H_{\text{on-site}},$$

where both layers have armchair edge. We further consider two different edge configurations as shown in left panel of Fig. 4 and 5, corresponding to different $H_{\text{int}}$. The band structure of $H_{\text{arm-arm}}^\uparrow(k_y, k)$ parameterized by $k_y$ is shown in right panel of Fig. 4 and 5, respectively, where the label $\uparrow$ represents the related $k_y$-parameterized bulk Hamiltonian is

$$H_{\text{arm-arm}}^\uparrow(k_y, k) = \eta^\dagger H_{\text{arm}}^\uparrow(k_y, k) \eta, \eta = (\xi_1, \xi_2)^T,$$

$$\xi_l = (b_{l,k}^a, a_{l,k}^a, a_{l,k}^f, b_{l,k}^f),$$

$$H_{\text{int}}^\uparrow(k_y, k) = \begin{bmatrix} h_{l,k}^a(k_y, k) & -H_{\text{int}}(k_y, k) \hline -H_{\text{int}}^\dagger(k_y, k) & h_{l,k}^f(k_y, k) \end{bmatrix},$$

which belongs to the non-trivial topological class $\mathcal{A}$ when there is no interlayer bias. When $U \neq 0$, it belongs to the trivial topological class $\mathcal{A}$.

For the BLG ribbon with the edge configuration shown in Fig. 4 there is no edge state even if non-zero $U$ and $\gamma_3$ are considered. For the edge configuration as shown in Fig. 5 the edge states which are gapped and flat appear when non-zero interlayer bias is added. Here we would like to point out that these edge states are not topological for three reasons: (i) They cannot be described by the bulk-edge correspondence used before since their energy is not at the Fermi level. (ii) They are not robust since they disappear when including $\gamma_3$, the quantity that preserves original chiral symmetry of the system and do not influence the existence of edge states in the case of bilayer bearded-bearded (zigzag-zigzag) ribbon (discussed below). (iii) Most importantly, they are not formed between two Dirac points with different topological charges in the band structure. But this fact is still interesting since it indicates the existence of edge states can be determined by interlayer bias.

### B. AB-stacked BLG with bearded-bearded (zigzag-zigzag) edges

The Hamiltonian that both layers have a bearded edge is analogous to the one with a zigzag edge. We take the one with the bearded edge as an example, whose Hamiltonian can be expressed as

$$H_{\text{bea-bea}} = \sum_i H_{\text{bea}}^i + H_{\text{int}} + H_{\text{on-site}}.$$

There are two different edge configurations, corresponding to different forms of $H_{\text{int}}$. Here these two types of Hamiltonians are denoted as $H_{\text{bea-bea}}^\leftrightarrow(k_y)$. Corresponding lattice structures are shown in Fig. 6(a) and (b), respectively. Meanwhile, $H_{\text{bea-bea}}^\leftrightarrow(k_y)$ are obtained by the
substitution: \( w \leftrightarrow v, a_{l,n} \leftrightarrow b_{l,n} \) in Fig. 6(a) and (b). The bulk Hamiltonian of the \( k_y \)-parameterized SSH ladder \( H_{\text{bea-bea}}(k_y) \) can be expressed as

\[
H_{\text{bea-bea}}(k_y) = \eta^\dagger h_{bb}(\gamma) (k_y, k) \eta,
\]

\[
\eta = (a_{1,k}, b_{1,k}, a_{2,k}, b_{2,k})^T,
\]

\[
h_{bb}(\gamma) (k_y, k) = \begin{bmatrix}
h_b^1(k_y, k) & H_{\text{int}}(\gamma) (k_y, k) \\
H_{\text{int}}(\gamma)(k_y, k)^\dagger & h_b^2(k_y, k)
\end{bmatrix},
\]

with

\[
h_b^1(k_y, k) = h_b(k_y, k) + \frac{(-1)^l}{2}U I_2, l = 1, 2,
\]

\[
H_{\text{int}}(k_y, k) = -\begin{bmatrix}
\gamma_3 e^{ik} \left( 2 \cos \frac{k_y}{2} + e^{ik} \right) & \gamma_1 \\
\gamma_1 e^{ik} \left( 2 \cos \frac{k_y}{2} + e^{-ik} \right) & 0
\end{bmatrix},
\]

which belongs to non-trivial class \( BDL \) only when \( U = 0 \), otherwise it belongs to trivial class \( AIII \) (Table. 1).

Unlike the armchair-armchair-edge case, the different geometry (distinguished by arrows) of bearded-bearded (zigzag-zigzag) edges of BLGs do not influence the band structure and edge states near the zero-energy (Fermi level). So we only show the band structure of bearded-bearded nanoribbon corresponding to \( H_{\text{bea-bea}}(k_y) \) in left panel of Fig. 4 for simplicity. The non-trivial and trivial topological classification straightforwardly determines the existence of zero-energy edge states since \( U \) breaks the chiral symmetry. The zero-energy edge states appear as flat fourfold degenerate bands when \( U = 0 \), belonging to non-trivial topological class. The related winding number calculation tells that they correspond to a winding number \( W = 2 \) when they are flat and \( W = 0 \) when they enter the bulk bands. Flat bands from each layer are separated by a gap when \( U \neq 0 \), as shown in Fig. 4. Bulk Hamiltonian of the SSH ladder \( H_{\text{bea-bea}}(k_y, k)(U \neq 0) \) belongs to topological trivial class (Table. 1). Here the edge states for \( U \neq 0 \) are still topological since they connect two topologically different Dirac points.\[6]

C. AB-stacked BLG with bearded-zigzag edges

Armchair MLG ribbon can only be stacked with armchair MLG ribbon to form an AB-stacked BLG ribbon. In contrast, zigzag MLG ribbon can be stacked with bearded MLG ribbon to form an AB-stacked BLG ribbon, which is described by the Hamiltonian

\[
H_{\text{bea-zig}}(k_y) = H_{\text{bea}(k_y)} + H_{\text{zig}(k_y)} + H_{\text{int}} + H_{\text{on-site}},
\]

Here we choose \( H_{\text{bea-zig}} \) as the example. The situation is the same as what we found in above subsection, where different edge configurations lead to similar band structures and related edge states near the zero-energy. Hamiltonians of different edge configurations can be denoted as \( H_{\text{bea-zig}}(k_y) \) as shown in Fig. 6(c) and (d), respectively. The bulk Hamiltonian of the SSH ladder \( H_{\text{bea-zig}}(k_y) \) can be expressed as

\[
H_{\text{bea-zig}}(k_y) = \eta^\dagger h_{\text{bea-zig}}(\gamma) (k_y, k) \eta,
\]

\[
\eta = (a_{1,k}, b_{1,k}, b_{2,k}, a_{2,k})^T,
\]

\[
h_{\text{bea-zig}}(k_y, k) = \begin{bmatrix}
h_b^1(k_y, k) & H_{\text{int}}(\gamma)(k_y) \\
H_{\text{int}}(\gamma)(k_y)^\dagger & h_b^2(k_y, k)
\end{bmatrix},
\]

FIG. 6. (Color online) The atomic structure of bearded-bearded ((a) and (b)) and bearded-zigzag ((c) and (d)) AB-stacked BLG ribbon in top view. The specific edge configuration is emphasized by the red box. The related \( k_y \)-parameterized SSH ladders are shown at the bottom, where (a)-(b) corresponds to \( H_{\text{bea-bea}}(k_y, k) \) and (c)-(d) corresponds to \( H_{\text{bea-zig}}(k_y, k) \), respectively. \( w = -2\cos(k_y/2) \) and \( v = -t \) are the same as used in Fig. 1.
When $U = 0$, $H_{\text{ber-zig}}(k_y)$ belongs to non-trivial class $BDI$. Otherwise, it belongs to trivial class $A2$ (Table. 1). The band structure of nanoribbon corresponding to $H_{\text{ber-zig}}(k_y)$ is plotted in right panel of Fig. 7. The twofold degenerate zero-energy edge state (flat band) can exist in the whole $k_y$ region when $U = 0$. It corresponds to a topological phase transition between two non-trivial topological phases characterized by $W = -1$ and $W = 1$ when crossing the Dirac point, as shown in left panel in Fig. 7. When $U \neq 0$, although the chiral symmetry is broken (i.e. no well-defined winding number), topological edge state still exists in the whole $k_y$ region with different energies when crossing the Dirac point. Notice that when $U \neq 0$, the bands are no longer twofold degenerate, as explained later.

This topological phase transition is not a numerical artifact. In contrast, it is protected by interlayer coupling. Winding number describes the mapping of Brillouin zone $(k)$ to $U(n)$ group, whose fundamental group is $Z^N$. In BLG ribbon case, it is $U(2)$. This mapping is orientation sensitive. For example, in calculating the winding number, $\gamma_3 = 0$ if $k_y$ is shown at the bottom. The reason for using $U \approx 0$ is explained in the text. Right panel: The distribution of the wave function $|\phi_1\rangle$ on different edges and different layers as a function of $k_y$ and the distribution of the wave function $|\phi_2\rangle$ in real space for two typical $k_y$ values with two different winding numbers. $n_{i=1,2}$ is site index on the respective layer, which increases along the finite direction of the ribbon. A transition between bottom-left and top-right is observed when crossing the Dirac point.

With

$$h_1(k_y, k) = h_z(k_y, k) - \frac{U}{2} \hat{l}_2,$$

$$h_2^z(k_y, k) = h_z^z(k_y, k) + \frac{U}{2} \hat{l}_2,$$

$$H_{\text{int}}(k_y) = -\begin{bmatrix} \gamma_3 \left(2 e^{i k} \cos \frac{k_y}{2} + 1\right) & 0 \\ 0 & \gamma_1 e^{i k} \end{bmatrix},$$

When $U = 0$, $H_{\text{ber-zig}}(k_y)$ belongs to non-trivial class $BDI$. Otherwise, it belongs to trivial class $A2$ (Table. 1). The band structure of nanoribbon corresponding to $H_{\text{ber-zig}}(k_y)$ is plotted in right panel of Fig. 7. The two-fold degenerate zero-energy edge state (flat band) can exist in the whole $k_y$ region when $U = 0$. It corresponds to a topological phase transition between two non-trivial topological phases characterized by $W = -1$ and $W = 1$ when crossing the Dirac point, as shown in left panel in Fig. 7. When $U \neq 0$, although the chiral symmetry is broken (i.e. no well-defined winding number), topological edge state still exists in the whole $k_y$ region with different energies when crossing the Dirac point. Notice that when $U \neq 0$, the bands are no longer two-fold degenerate, as explained later.

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The non-zero winding number of it can be turned into $-2$ instead of 2 by reversing the direction of $k$. In the BLG bea-zig case, as in the right panels of Fig. [7] it is the bearded layer/zigzag layer that is responsible for the $1/2$ part of winding number. If we can choose the orientation of $k$ independently for each layer, we can make the winding number always 1, i.e. no phase transition is present. This simple conjecture can be verified by setting $\gamma_3 = \gamma_1 = 0$, i.e. two decoupled ribbon. In that case, one can indeed find a chiral operator $S$ such that the calculated winding number is always 1 (or always $-1$). For example, it can be done by using $S = \text{diag}(1, -1, 1, -1)$ for the Hamiltonian in Eq. (19) with $\gamma_3 = \gamma_1 = 0$. It is permissible for an uncoupled system to have different orientation of Brillouin zone for each subsystem. However, the presence of interlayer coupling, which is present in the real BLG system, prohibits us from choosing the orientation of $k$ independently for each layer. We are forced to choose the same orientation of $k$ for two layers of ribbon. Otherwise, we are not able to write $H_{int}$ in Bloch form. More specifically, this means that $S = \text{diag}(1, -1, 1, -1)$ is no longer a chiral symmetry operator for Eq. (19) with non-zero interlayer coupling. In this sense, the observed topological phase transition is protected by interlayer coupling.

The change in winding number can be seen from the behavior of the wave function of edge states. For $W = 1$ ($|v| < |w|$) region, one of the degenerate edge states can be approximately expressed as

$$|\varphi_1\rangle \approx \frac{1}{\sqrt{\Omega_1}} \sum_{j=1}^{N} \left( -\frac{w}{v} \right)^{N-j} b_{1,j} \left| 0 \right>,$$

$$\Omega_1 = \frac{1 - (w/v)2N}{1 - (w/v)^2} \approx \frac{w^2}{w^2 - v^2},$$

for $\gamma_3 = U \approx 0$, which is equivalent to one of the edge states of MLG ribbon with bearded edges (bottom layer), as shown in Fig. 8, where the label $l = 1, 2$ in $a_{1,j} \left| b_{1,j} \right>$ represents the bottom/top layer respectively. The other edge state is

$$|\varphi_2\rangle \approx \frac{1}{\sqrt{\Omega_2}} \sum_{j=1}^{N} \left( -\frac{w}{v} \right)^{j-1} a_{1,j} \left| 0 \right>$$

$$+ \left( -1 \right)^j \left( -\frac{w}{v} \right)^{j-1} a_{2,j} \left| 0 \right>,$$

$$\Omega_2 = \frac{1 - (v/w)2N}{1 - (v/w)^2} + \left( \frac{w}{v} \right)^2 \sum_{j=1}^{N} j^2 \left( \frac{v}{w} \right)^{2j-2}$$

$$\approx \frac{w^2}{w^2 - v^2} + \frac{w^2}{v^2 - w^2}.$$
It turns out the difference between these two edge configurations appears in the form of non-topological edge states, as discussed below.

Besides the topological edge states we discussed in the last section, which exist as gapless or gapped flat bands near the zero energy (Fermi level), some unexpected edge states are found in the gap within bulk bands that are away from the zero energy (Fermi level) in the AB-stacked BLGs with a bearded-bearded (zigzag-zigzag) edge or a bearded-zigzag edge, as shown in Fig. 9.
provide 4 energy levels as shown in Fig. 10(a). Each 4-site structure would the simply repeated decoupled 4-site structures

\[ H_{\text{bea-bea}}(k_y = \pi) \]

with \( \gamma_3 = 0 \), describes the simply repeated decoupled 4-site structures

\[ h_4 = w_{eq}c_1^{\dagger}c_2 + v_{eq}c_2^{\dagger}c_3 + w_{eq}c_3^{\dagger}c_4 + \text{H.c.} + \sum_{j=1}^{2} \frac{(-1)^{j+1}}{2} \left( c_{2j-1}^{\dagger}c_{2j-1} + c_{2j-1}c_{2j}^{\dagger} \right) , \]

as shown in Fig. 10(a). Each 4-site structure would provide 4 energy levels

\[ E = \pm \frac{1}{2} \sqrt{2\gamma^2 + U^2 + 4t^2 \pm 2\varepsilon} , \]

(26)

\[ \varepsilon = \sqrt{4U^2t^2 + 4t^2\gamma^2 + \gamma^4} , \]

and each of these four energy levels are highly degenerate since there are many identical 4-site structures. When we consider the region close to \( k_y = \pi \), each of the four highly degenerate levels would split into many bulk states according to first order degenerate perturbation theory. So there are no edge states under this scenario in the neighbour of \( k_y = \pi \) in the bulk gap.

If \( \gamma_3 \approx \gamma_1 \) as we discussed before, the energy bands of \( H_{\text{bea-bea}}(k_y = \pi) \) is dominated by not only a simply repeated decoupled 4-site structure but also a newly formed SSH chain

\[ h_{\text{SSH}} = \sum_{n=1}^{N} w_{eq}a_n^{\dagger}b_n + v_{eq}b_n^{\dagger}a_{n+1} + \text{H.c.} + \sum_{n=1}^{N} \frac{(-1)^{n+1}}{2} U \left( a_n^{\dagger}a_n + b_n^{\dagger}b_n \right) , \]

as shown in the Fig. 10(a). Because \( t \gg \gamma_1 \) in our choice of parameter, \( h_{\text{SSH}} \) is general in most cases, this equivalent SSH chain leads to no edge states. This is in accord with the results shown in both Fig. 7 and Fig. 9(a).

However, the situation is different for \( H_{\text{bea-bea}}'(k_y) \). When \( \gamma_3 = 0 \), two isolated 2-site structures

\[ h_2 = w_{eq}c_1^{\dagger}c_2 + \text{H.c.} + \frac{U}{2} \left( c_1^{\dagger}c_1 + c_2^{\dagger}c_2 \right) , \]

(28)

appear in addition to repeated decoupled 4-site structures, as shown in Fig. 10(b). These isolated 2-site structures provide the eigenstates with energy \( \pm U/2 \pm t \), as shown in Fig. 9(b). When we consider the region close to \( k_y = \pi \), since the energy of 2-site structure is different from (well separated) that of bulk 4-site structure, their eigenstates would predominantly mix among themselves instead of mixing with states from those 4-site structures. Since these two 2-site only exist at the edge, the mixing result would remain edge states. If \( \gamma_3 \approx \gamma_1 \), two equivalent SSH chains exist as shown in Fig. 10(b). Each of these chains is the same as the structure of \( h_{\text{SSH}} \), leading to no edge states both near the zero energy (Fig. 7) and in the gap within bulk bands (Fig. 9(b)).

The condition is more complicated when we discuss the AB-stacked BLGs with a bearded-zigzag edge. For \( H_{\text{bea-zig}}'(k_y = \pi) \) with \( \gamma_3 = 0 \), the same two isolated 2-site structures at the end of chain and repeated decoupled 4-site structure appear as in previous cases. Besides, there are also an isolated 1-site \( h_1 = (U/2) c_1^{\dagger}c_1 \) and a 3-site structure at two ends of chain

\[ h_3 = w_{eq}c_1^{\dagger}c_2 + v_{eq}c_1^{\dagger}c_3 + \text{H.c.} - \frac{U}{2} \left( c_1^{\dagger}c_1 + c_2^{\dagger}c_2 - c_3^{\dagger}c_3 \right) , \]

as shown in Fig. 10(c). The two edge states near zero energy are from \( h_1 \) and one of eigenstates of \( h_3 \) with close-to-zero energy. The three edge states appearing in the gap within bulk bands shown in Fig. 9(c) are naturally described by one eigenstate of \( h_3 \) with \( E \approx 0 \) and two eigenstates of two \( h_2(U = 0) \) with energy \(-t\). Again, in the neighbourhood of \( k_y = \pi \), states from 1-site/2-site/3-site will mix among themselves instead of mixing with bulk 4-site states due to energy difference. Thus these states would remain edge states in this neighbourhood. When \( \gamma_3 \approx \gamma_1 \), two SSH chain structures appear with odd number of sites, each of them provides one edge state near zero energy. All other states of odd-site SSH chain are bulk states. Thus, there are no edge states in the gap within bulk bands, as shown in Fig. 9(c).

At last we discuss \( H_{\text{bea-zig}}'(k_y = \pi) \). \( \gamma_3 = 0 \) leads to the repeated decoupled 4-site structures, one isolated 1-site, and one 3-site structures as shown in Fig. 10(d). The edge state shown in Fig. 9(d) comes from one eigenstate of \( h_3 \) with \( E < 0 \). The two near-zero edge states are eigenstate of \( h_1 \) and one of eigenstates of \( h_3 \). If \( \gamma_3 \approx \gamma_1 \), two SSH chains structures appear with odd number of sites. Together they provide two zero-energy edge states, and no edge states in the gap within bulk bands, as shown in Fig. 9(d).

As a conclusion, number of edge states away from Fermi-energy is determined by the number of isolated structures when \( k_y = \pi \), which is in turn dependent upon the edge configuration of AB-stacked BLGs.

V. CONCLUSIONS AND DISCUSSIONS

In this paper, we discussed the existence and topology of edge states in AB-stacked BLG ribbon with various edge configurations. We illustrated the correspondence between BLG ribbon and SSH ladder. A detailed topological classification based on discrete symmetry and
energy edge state existing in the whole two topologically non-trivial phases in zigzag-bearded.

We also found a topological phase transition between two topologically non-trivial phases in zigzag-bearded BLG ribbon, corresponding to a twofold degenerate zero-energy edge state existing in the whole $k_y$ region. We demonstrated that when a edge state crosses the phase transition point, it will switch both layer and edge.

Moreover, we pointed out that some non-topological edge states without the protection of the chiral symmetry can be found in the gap within bulk bands that are away from zero-energy (Fermi level). The existence and number of these states are sensitive to the edge configurations of BLG ribbons even if their bulk topologies are the same, which can be simply explained by effective Hamiltonians $H(k_y = \pi)$ for different situations. Though we focus only on the honeycomb lattice in this paper, it should be obvious that our study can be generalized to lattices of different shapes, such as Kagome and triangular lattices, and of higher dimensions, such as the description of edge states and surface states in three dimensional topological insulators. All of these provide potential directions for further study.

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Appendix: The difference between wave vector number $k_y$ and $k$

The following example is provided to make the discussion in section 1 of the main text more concrete. Consider the ribbon depicted in Fig. 1(a), the Hamiltonian is given by Eq. (2) of the text:

$$H_{\text{bea}} = -t \sum_{m=1}^{M} \sum_{n=1}^{N} \left[ a_{m,n}^\dagger b_{m,n} + b_{m,n}^\dagger a_{m,n+1} + b_{m,n}^\dagger b_{m+1,n+1} \right] + H.c. \right)$$ (A.1)

For this specific ribbon, $N = 5$. The value of $M$ is unimportant since the ribbon is infinite (periodic) along that direction. It is a common practice to assume that there is a periodicity in the operator, i.e. $a_{i,j}^{(t)} = a_{i+M,j+N}$ and $b_{i,j}^{(t)} = b_{i+M,j+N}$. Notice that under this condition, the Hamiltonian given by Eq. (2) is invariant when adding 1 to all the first subscript of all operators. But it is not invariant when adding 1 to all operators’s second subscript. This difference is due to the term $b_{m,N}^\dagger (a_{m,1} + a_{m+1,1})$, hence we say that this term gives the open boundary condition.

By basic solid state physics, we are allowed to make Fourier transformation along the invariant direction, which is the direction of the first subscript. The Fourier transformation is given by Eq. (3) of the main text, while the resulting Bloch form Hamiltonian is given by Eq. (4).

Consider now doing the following redefinition of operators, which is always allowed since it does not affect the band structure.

$$a_{k_y,n}^\dagger \rightarrow a_{k_y,n}^\dagger e^{i k_y n/2},$$ (A.2)

$$b_{k_y,n}^\dagger \rightarrow b_{k_y,n}^\dagger e^{i k_y n/2}$$

After this redefinition, the Hamiltonian in Eq. (4) will be transformed into the form of Eq. (5), which is the following, where $a_{k_y,n} / b_{k_y,n}$ are shorthand for $a_{k_y,n}/b_{k_y,n}$

$$H_{\text{bea}}(k_y) = \sum_{n=1}^{N} \left( v a_{k_y,n}^\dagger b_{n} + w b_{k_y,n}^\dagger a_{n+1} + v a_{k_y,n}^\dagger b_{N} + H.c. \right)$$ (A.3)

From this point on, we will leave MLG ribbon, and instead consider a 10-site SSH chain as illustrated in Fig. 11. Its intercell coupling $w$ and intracell coupling $v$ are defined as following:

$$v \equiv -t \quad w \equiv -2t \cos(\frac{k_y}{2})$$ (A.4)

Readers should refrain from associating $k_y$ appearing above with the one obtained in the Fourier transformation of MLG ribbon, but instead should think it just as a parameter on which $v$ and $w$ depend. The Hamiltonian of the 10-site SSH chain is:

$$H_{\text{dimer}} = \sum_{n=1}^{N} \left( v a_{k_y,n}^\dagger b_{n} + w b_{k_y,n}^\dagger a_{n+1} + v a_{k_y,n}^\dagger b_{N} + H.c. \right)$$ (A.5)

$H_{\text{dimer}}$ is formally equivalent to $H_{\text{bea}}(k_y)$, i.e. $H_{\text{dimer}} \cong H_{\text{bea}}(k_y)$. However, it is more obvious that this is an additional trick we can play with this 10-site SSH chain. We can make this chain infinite and obtain a Hamiltonian $H_{\text{chain}}$ that can be put in Bloch form, with corresponding Bloch wave vector $k$, as used in the main text.

$$H_{\text{infinite chain}} = \sum_{k \in FBZ} H(k)$$

$$H(k) = \begin{pmatrix} v + we^{-ik} & a_{k_y}^\dagger b_{k} + H.c. \\ 0 & v + we^{ik} \end{pmatrix}$$ (A.6)
This $H(k)$ is dependent on $k_y$ through $v$ and $w$. This $H(k)$ is what is referred to as $h_0(k_y, k)$ in Eq. (6) of the text, with which we can calculate winding number $W$ for different $k_y$ using Eq. (7) and Eq. (8) of the text. For this specific example, the chiral operator $S$ is

\[
S = \begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}
\]  

(A.7)

This procedure can be easily generalized to bilayer case as we use in later sections.

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64 The presence of these edge states is still dependent on edge configuration, since only one of the two edge configurations of BLG arm–arm ribbon show them. However, the mechanism itself, i.e. bias, does not treat the atoms on the edge differently from those deep inside the bulk. This is different from edge states induced by modulating only the edge onsite energy. More specifically, after we impose this bias, the effective $k_y$ parameterized SSH ladder for BLG arm–arm ribbon still has a bulk Hamiltonian, on which we can discuss the topology. However, if we only modulate the onsite energy on the edge of BLG arm–arm ribbon, the effective SSH ladder does not have a bulk Hamiltonian.