Low-energy Landau levels of Bernal zigzag graphene ribbons

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Low-energy Landau levels of Bernal zigzag graphene ribbons in the presence of a uniform perpendicular magnetic field (B) are investigated by the Peierls coupling tight-binding model. State energies and associated wave functions are dominated by the B-field strength and the kz-dependent inter-ribbon interactions. The occupied valence bands are asymmetric to the unoccupied conduction bands about the Fermi level. Many doubly degenerate Landau levels and singlet curving magnetobands exist along the kx and kz directions, respectively. The kz-dependent inter-ribbon interactions dramatically modify the magnetobands, such as the lift of double degeneracy, the change in state energies, and the production of two groups of curving magnetobands. They also change the characteristics of the wave functions and cause the redistribution of the charge-carrier density. The kz-dependent wave functions are further used to predict the selection rule of the optical transition. © 2009 American Institute of Physics. [DOI: 10.1063/1.3159643]

I. INTRODUCTION

Carbon-based materials, such as graphite, carbon nanotubes,1 two-dimensional (2D) graphene and few-layer graphenes,2–5 and graphene ribbons, have been widely studied both experimentally and theoretically. Graphene ribbons could be synthesized by using heat treatment,6–8 pulsed-laser deposition technique,9 patterning epitaxially grown graphenes,10,11 tailoring exfoliated graphenes12,13 by scanning tunneling microscopy,14 or chemical vapor deposition.15 A one-dimensional (1D) graphene ribbon is obtained by cutting a 2D graphene, planar hexagonal lattices of carbon atom, along the longitudinal direction. As a result of the special geometric structure, graphene ribbons have motivated many interesting studies on magnetic properties,16–20 optical properties,19–21 electronic excitations,22 or electronic properties.23 The objective of this work is to investigate the magnetoelectronic structures of Bernal graphene ribbons.

1D zigzag and armchair graphene ribbons, sided with two parallel zigzag and armchair structures along the longitudinal direction, respectively, are intensively studied. Many theoretical studies predict that a zigzag ribbon has peculiar edge states. Such edge states produce flatbands at low energy and give rise to a conspicuous peak in the density of states.24 An armchair ribbon does not exhibit such states. Its electronic properties, such as the band gap, depend on the ribbon width. Furthermore, 2D multilayer zigzag (armchair) graphene ribbons are the stack of infinite identical 1D zigzag (armchair) graphene ribbons along the stacking direction (Fig. 1). This stacked system exhibits the anisotropic energy dispersions between in-ribbon plane and the stacking direction for the intraribbon coupling is much stronger than the inter-ribbon interaction. Moreover, the inter-ribbon interactions also modify the in-ribbon plane electronic properties, such as state energies, energy dispersions, band-edge states, and size of band gap. The study results show that the geometrical structures [the stacking types (AA or AB stacking),

FIG. 1. (Color online) (a) The geometric structure of the N\textsubscript{z}=3 Bernal zigzag graphene nanoribbons. (b) γ\textsubscript{0}=2.598 eV is the intralayer interaction, γ\textsubscript{1}=0.364 eV (γ\textsubscript{2}=0.036 eV) represents the interaction between two A atoms from two neighboring ribbons (two next-neighboring ribbons), and γ\textsubscript{3}=0.319 eV (γ\textsubscript{4}=−0.014 eV) is for B atoms. γ\textsubscript{5}=0.177 eV corresponds to the inter-ribbon interaction between A atoms and B atoms. γ\textsubscript{6}=−0.026 eV is the chemical shift between A atoms and B atoms. The values of γ\textsubscript{i} are the same as those of Bernal graphite (Ref. 38).

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ribbon width, and ribbon edge structure] have a significant effect on the electronic and optical properties of multilayer graphene ribbons.25–27 The optical measurement might serve as a method to determine the geometrical structures of graphene ribbons.28

When a monolayer graphene ribbon is submitted to a perpendicular magnetic field \(B\), its magnetoelectronic properties, e.g., the magnetic bands and the related wave functions, are determined by the competition between the magnetic confinement and the quantum confinement.19,20,29 When the spatial extent of Landau wave functions is smaller than the ribbon width, i.e., the magnetic confinement predominates over the quantum confinement, the Landau states exist and the state energy follows
\[
E = \frac{\hbar^2}{2m} \frac{1}{N^2} \sum_{j} \langle c^+_j | H | c^+_j \rangle + \text{H.c.},
\]
(1)

where the subindices \(i\) and \(j\) denote the summation over all sites in a primitive unit cell. \(c^+_j\) is the creation (annihilation) operation, which generates (destroys) an electron at \(i\) (\(j\)) site. The details of the atom-atom interactions38 \(\gamma_{i,j} = \gamma_{0,1,\ldots,\gamma_{6}}\) are described in Fig. 1(b). \(e^{i2\pi h_{ij}}\) is the Peierls phase shift due to the applied magnetic field. \(\theta_{ij}\) is the line integral of vector potential \(A\) from \(i\) to \(j\) in a unit of the flux quantum \(\Phi_0 = ch/e\). To keep the translation invariance along the \(x\) axis, within the Landau gauge, the vector potential \(A = -(By,0,0)\) is deliberatively adopted. In this gauge, Bernal zigzag ribbons have two ribbons or \(4N_c\) carbon atoms in a primitive cell. The first Brillouin zone is a rectangle defined by \(-\pi/N_c \leq k_x = \pi/N_c\) and \(-\pi/2l_c \leq k_z \leq \pi/2l_c\), where \(l_c\) is the stacking distance of the two \(ABAB\) sequences along the \(z\) axis.

The tight-binding Bloch function is the linear combination of bases \(|A_{m1}\rangle, |B_{m1}\rangle, |A_{m2}\rangle, \text{ and } |B_{m2}\rangle\), which are the linear superposition of the \(2p_z\) orbitals located at \(A_{m1}, B_{m1}, A_{m2}, \text{ and } B_{m2}\) carbon atoms. The wave function is
\[
|\Phi(k_x,y,k_z)\rangle = \sum_{m=1}^{N_c} a_{A_{m1}}|A_{m1}\rangle + b_{B_{m1}}|B_{m1}\rangle + \sum_{m=1}^{N_c} a_{A_{m2}}|A_{m2}\rangle + b_{B_{m2}}|B_{m2}\rangle,
\]
(2)

where wave function coefficients \(a_{A_{m1}}, b_{B_{m1}}, a_{A_{m2}}, \text{ and } b_{B_{m2}}\) are the site amplitudes.

The Hamiltonian representation is a \(4N_c \times 4N_c\) Hermitian matrix and could be regarded as
\[
H = \begin{bmatrix} h_{11} & h_{12} \\ h_{12} & h_{22} \end{bmatrix},
\]
(3)

where each Hermitian block matrix \(h_{11}, h_{12}, h_{12}, \text{ or } h_{21}\) has \(2N_c \times 2N_c\) elements. The block matrix \(h_{11}\), Hamiltonian representation of the lower ribbon, is a tridiagonal matrix and its matrix elements \(h_{1(i,j)}\) are
\[
h_{1}(1,2-m-1) = \gamma_6 + \beta^2 \gamma_3/2,
\]
\[
h_{1}(2,2m) = \beta^2 \gamma_2/2,
\]
\[
h_{1}(2m,2m-1) = h_{1}(2m,2m-1) = 2 \gamma_0 \cos \left( \sqrt{3} h k_{z}/2 - \pi (m - [N]) \Phi \right),
\]
\[
h_{1}(2m,2m+1) = h_{1}(2m,2m+1) = \gamma_6,
\]
(4)

where \(m=1,2,\ldots,N_c\) and \(\beta=2 \cos(k_{l} l_c)\). \([N]=([N]+1)/2\) is used to locate the origin of coordinate in the center of the

II. THEORY

The Bernal zigzag graphene ribbon is chosen for the model study. It has hydrogen-terminated zigzag edges along the longitudinal (\(\bar{x}\)) direction [Fig. 1(a)]. The ribbon width is defined by the number \(N_c\) of zigzag lines along the \(y\) axis. \(B\) and \(A\) atoms are different sublattices of biparticle hexagonal lattice of a graphene ribbon. There are \(2N_c\) carbon atoms in a primitive cell of a monolayer graphene ribbon. To obtain the 2D Bernal zigzag graphene ribbon, the same 1D zigzag

ribbons are piled in the \(ABAB\) sequence along the \(z\) axis with the stacking distance \(l_c=3.35\ \text{Å}\). The \(A\) atoms have the corresponding atoms on the \(x-y\) plane directly above or below them, while the projections of the \(B\) atoms are located at the center of the hexagonal rings directly above or below them [Fig. 1(b)].

In the presence of a perpendicular magnetic field \(B = (0,0,B)\), the electronic properties of Bernal zigzag ribbons are modeled by the Peierls coupling tight-binding model. The Hamiltonian is
\[
H = \sum_{i,j} \left( \gamma_{i,j} e^{i2\pi \theta_{ij}/[c^+_i c^-_j] + \text{H.c.}} \right),
\]
where the subindices \(i\) and \(j\) denote the summation over all sites in a primitive unit cell. \(c^+_i\) is the creation (annihilation) operation, which generates (destroys) an electron at \(i\) (\(j\)) site. The details of the atom-atom interactions38 \(\gamma_{i,j} = \gamma_{0,1,\ldots,\gamma_{6}}\) are described in Fig. 1(b). \(e^{i2\pi h_{ij}}\) is the Peierls phase shift due to the applied magnetic field. \(\theta_{ij}\) is the line integral of vector potential \(A\) from \(i\) to \(j\) in a unit of the flux quantum \(\Phi_0 = ch/e\). To keep the translation invariance along the \(x\) axis, within the Landau gauge, the vector potential \(A = -(By,0,0)\) is deliberatively adopted. In this gauge, Bernal zigzag ribbons have two ribbons or \(4N_c\) carbon atoms in a primitive cell. The first Brillouin zone is a rectangle defined by \(-\pi/N_c \leq k_x = \pi/N_c\) and \(-\pi/2l_c \leq k_z \leq \pi/2l_c\), where \(l_c\) is the stacking distance of the two \(ABAB\) sequences along the \(z\) axis.

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h_{1}(2m,2m+1) = h_{1}(2m,2m+1) = \gamma_6,
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where \(m=1,2,\ldots,N_c\) and \(\beta=2 \cos(k_{l} l_c)\). \([N]=([N]+1)/2\) is used to locate the origin of coordinate in the center of the

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ribbon. $\pi\Phi$, the Peierls phase shift, results from the magnetic flux passing half a hexagonal ring. The diagonal term $\gamma_0 + \beta^2 \gamma_2/2$ due to the inter-ribbon interactions, can be treated as the equivalent site energy of $A$ ($B$) atoms. The centers of the two ribbons in a unit cell do not coincide with each other [Fig. 1(a)]. This leads to a different tridiagonal matrix $h_2$, which is

$$h_2(2m - 1, 2m - 1) = \gamma_0 + \beta^2 \gamma_2/2,$$

$$h_2(2m, 2m) = \beta^2 \gamma_2/2,$$

$$h_2(2m - 1, 2m - 2) = h_2(2m, 2m - 2) = \gamma_0.$$  \label{eq:5}

The term $\pi\Phi/3$ in Eq. (5) is caused by the difference between the centers of the two ribbons in a unit cell.

The two off-diagonal block matrices satisfy a simple relation $h_{12} = h_{21}$. As a result of the inter-ribbon interactions, the nonzero matrix elements $h_{12}(i, j)$ of the off-diagonal block matrix $h_{12}$ are as follows:

$$h_{12}(2m - 1, 2m - 1) = \beta \gamma_1,$$

$$h_{12}(2m, 2m) = \beta \gamma_3,$$

$$h_{12}(2m - 1, 2m - 2) = \beta \gamma_4,$$

$$h_{12}(2m, 2m - 2) = \beta \gamma_4.$$  \label{eq:6}

The effect of magnetic fields is reflected in the interaction $2 \gamma_i \cos(\sqrt{3}bk_i/2 - \pi(m - [N])\Phi)$. All the nonzero elements of $h_{12}$ depend on $\beta = 2 \cos(k_L)$. The inter-ribbon interactions are equal to zero at $k_L \pi = \pi/2$, and they are maximum at $k_L \pi = 0$. Eigenvalues and eigenvectors are obtained after the diagonalization of the Hamiltonian matrix. Eigenvalues are the energy dispersions $E^c(\kappa, k_c, k_L)$, where $c$ ($\nu$) represents the unoccupied (occupied) states. The eigenvector $|\psi^{\nu}(x, y, k_L)\rangle$ is the $k_c$-dependent envelope function $|\psi^{\nu}(y, k_c)\rangle$ along the $y$ direction.

### III. MAGNETOELECTRONIC PROPERTIES

The band structures of the 2D multilayer graphene ribbons exhibit a highly anisotropic structure. Figures 2(a)–2(c) show the $k_c$-dependent low-energy bands for the Bernal zigzag graphene ribbon with width $N_z = 3000$ (639 nm) at $B = 0$, $B = 20$ T, and $B = 10$ T, respectively. The unit of energy is eV. The Fermi level is set to $E_F = 0$. At $B = 0$, the low-energy bands are similar to those obtained from the local density approximation calculations. These bands include parabolic bands and flatbands [Fig. 2(a)]. The occupied valence bands are asymmetric to the unoccupied conduction bands about $E_F$ due to the energy-dependent inter-ribbon interactions. The $N_z = 3000$ Bernal zigzag graphene ribbon is a semimetal because the valence bands tightly touch the conduction bands at $E_F = 0$. The degeneracy of the flatbands at $E = 0$, a special feature of a single zigzag ribbon due to the zigzag-edge boundaries, is lifted by the inter-ribbon interactions. The partial flatbands near $E_F = 0$ correspond to the edge states mainly localized at the outmost zigzag positions. According to Figs. 2(b)–2(d), the magnetic field drastically modifies the energy bands, such as the alteration of the band feature, the shift of the subbands, and the production of the Landau levels. At $B = 20$ T, as shown in Fig. 2(b), the original parabolic bands might become the complete Landau levels. The occupied states $E^c$ are asymmetric to the unoccupied states $E^a$ about $E_F = 0$. The Landau-level energies do not follow the simple relation $E \approx \sqrt{n}\hbar$. The presence of $B$ induces a longer and weak splitting energy subband near $E_F$, namely, the zero mode. There are more Landau subbands and a shorter range in band structure as the magnitude of the magnetic field decreases [Fig. 2(c)]. The zigzag boundaries make narrow graphene ribbons exhibit special electronic and magnetic properties.40,41

Interestingly, the inter-ribbon interactions induce the concave-upward and concave-downward magnetobands.
The energy dispersions near $E_F$ at $B=20$ T with $N_c=3000$, $B=10$ T with $N_c=3000$, and $B=20$ T with $N_c=6000$ (1278 nm) along the $k_z$ axis are shown in Figs. 2(e)–2(h), respectively, to illustrate the effect of inter-ribbon interactions. There are oscillating subbands, concave-upward and concave-downward bands, and nearly dispersionless bands nearby $E_F$ [Figs. 2(e) and 2(f)]. The occupied states $E^-$ are asymmetric to the unoccupied states $E^+$ about $E=0$. The main feature of the energy dispersions remains unchanged for the variation of magnetic flux. However, the state energies are sensitive to the magnitude of the magnetic field [Fig. 2(g)]. The zero mode near $E_F$, including two oscillating subbands, has a dispersion of 0.04 eV at the low field limit.

The upper subband of the zero mode, indexed by $n=0$, shows the cosine energy bands $E=\cos(k_z L/2)$ along the $k_z$ directions, while the feature of the lower subband, indexed by $n'=0$, is distorted. A pseudogap $\Delta$ associated with the zero mode near $E_F$ is observed. Thus, the size of the pseudogap $\Delta$ varies with $k_z$. The upper limit of the pseudogap $\Delta$, occurring at $k_z L/2=\pi/2$, is equal to $\gamma_0$, the chemical difference between $A$ atoms and $B$ atoms. The concave-upward and concave-downward subbands are classified into two groups. One group, denoted as group I, moves towards $E_F$ while the other, group II, moves away from $E_F$. The first three subbands of each group are shown in Fig. 2(f) as examples. The unoccupied states $E^-$ and occupied states $E^+$ of group I are denoted by subband indices $n$ and $n'$, respectively. Those of group II are indexed, respectively, by $\bar{n}$ and $\bar{n}'$. The subband crossings occur at different $k_z$. The band-edge states, the local minimum and maximum, of the $n$, $\bar{n}$, and $\bar{n}'$ subbands are located at $k_z=0$.

The Landau plot, the Landau-level energies versus the field strength, at different $k_z$ can reveal the effect of the inter-ribbon interactions. The Landau plot of the $N_c=3000$ Bernal zigzag ribbon at $k_z L/2=\pi/2$ is shown in Figs. 3(a) and 3(b). The state energies of the zero mode are independent of the field strength. The energy spacing between the upper and lower subbands, the pseudogap $\Delta$ at $k_z L/2=\pi/2$, is equal to $\gamma_0$. Except for the zero mode, Landau-level energies follow the simple relation $E_n=\sqrt{n}\gamma B$. The chief reason is that the two ribbons in a primitive unit cell are regarded as two independent ribbons because the inter-ribbon interactions are turned off at $k_z L=\pi/2$. The magnetoelectronic properties are dominated by the magnetic confinement rather than the quantum effect. Accordingly, the Landau-level energies, indexed by $n$, follow the relation $E_n=\sqrt{n}\gamma B$. On the other hand, the inter-ribbon interactions between the two ribbons are maximum at $k_z L=0$. The Landau plots, as shown in Figs. 3(c) and 3(d), exhibit different behaviors. The state energies of the zero mode vary with the field strength. In the energy region $|E|<0.02\gamma_0$, the state energies of the first and second unoccupied (occupied) Landau levels exhibit the linear-in- $B$ dependence at $B \approx 50$ T. The high-energy Landau levels, indexed by $n \geq 3$, exhibit the linear-in-$B$ dependence at $B \approx 15$ T. Then, they evolve from a linear-in-$B$ dependence to a square-root $B$ dependence with the increase in the field strength. Finally, they exhibit the linear-in-$\sqrt{B}$ dependence at $B \approx 20$ T.

The effect of inter-ribbon interactions on the envelope functions deserves a closer examination. Envelope functions of the $N_c=3000$ zigzag ribbon subjected to $B=20$ T at different $k_z$ are shown in Figs. 5(a)–5(d). Each envelope function $\Psi(y,k_z)$ is separated into eight components, $\psi(A_{n1}^1)$, $\psi(A_{n2}^1)$, $\psi(A_{n3}^1)$, $\psi(A_{n4}^1)$, $\psi(B_{n1}^1)$, $\psi(B_{n2}^1)$, $\psi(B_{n3}^1)$, and $\psi(B_{n4}^1)$. $A_n^1$ and $B_n^1$ denote $A$ and $B$ atoms located at the odd (even) zigzag lines at the lower (upper) ribbon plane. The subenvelope function $\psi(A_{n1}^1)$, for example, is $[a_{n1},a_{n1},a_{n1},...]$. Because $\psi(A_{n1}^1)=-\psi(A_{n1}^1)$, $\psi(B_{n1}^1)=-\psi(B_{n1}^1)$, $\psi(A_{n2}^1)=-\psi(A_{n2}^1)$, and $\psi(B_{n2}^1)=-\psi(B_{n2}^1)$, only four components, $\psi(A_{n1}^1)$, $\psi(B_{n1}^1)$, $\psi(A_{n2}^1)$, and $\psi(B_{n2}^1)$, are displayed. The evolution of wave functions with $k_z$ is deliberated.

At $k_z L/2=\pi/2$, the inter-ribbon interactions are closed due to $B=2\cos(k_z L)=0$ [Eqs. (4)–(6)]. The two ribbons in a primitive unit cell are decoupled, i.e., there are two isolated graphene ribbons. Except for the zero mode, the state energies are double degenerate. Their associated envelope functions, $\Psi_1(y,k_z L=\pi/2)$ and $\Psi_2(y,k_z L=\pi/2)$, are orthogonal to each other and different in the sign of some components. One of the two envelope functions is shown in Fig. 4(a). It is exactly described as $[\phi_0(A_{1}^1),\phi_{n-1}(B_{1}^1),\phi_{n-1}(A_{1}^1),\phi_{n-1}(B_{1}^1)]$, where $\phi_0$ is the harmonic oscillator, product of the Hermite polynomial $H_{n}$ and the Gaussian function. Each $\phi_n$ has $n$ nodes, where the subenvelope function changes the signs. The node number $n$ of the subenvelope function $\psi_n(A_{1}^1)$ is identical to the subband index $n$. Thus, we use the subband indices $n=1,2,...$ and $n'=1,2,...$ to specify the characteristic of the envelope function [Fig. 4(a)]. $\phi_0(A_{1}^1)$ and $\phi_n(B_{1}^1)$
[\phi_{n,1}(B^1_0)] and [\phi_{n,1}(A^2_0)] belong to the n (n-1) mode. The envelope functions are the same as those of a single graphene ribbon. Due to the orthogonality, \Psi_n and \Psi_n', are different in the sign of some components. Besides, \Psi_n=\phi_0(B^0_e) - \phi_0(B^0_e)', the envelope function of the n=0 subband, is located in the B sites of the upper ribbon. \phi_0(A^1_e) - \phi_0(A^1_e)', the envelope function of the n'=0 subband, is mainly controlled by the A atoms on the lower ribbon plane. The chemical difference \gamma_6 changes the site energies of atoms A, and thus causes the energy split and produces a pseudogap \Delta=\gamma_6 between \Psi_n=0 and \Psi_n'=0 at k_z = \pi/2 [Fig. 2(e)].

Away from k_z = \pi/2, the switched-on inter-ribbon inter-
actions not only produce two groups of subbands but also change the aspects of envelope functions. At \(k \cdot I_\perp = 0.499 \pi\), the envelope functions related to \(n\) and \(\bar{n}\) subbands concentrate on the lower and upper ribbons, respectively [Fig. 4(b)]. The envelope functions are, respectively, \(\{\psi_{n=1}(A_1^\perp), \psi_{n=1}(B_1^\perp), 0, 0\}\) and \(\{0, 0, \psi_{n+1}(A_1^\perp), \psi_{n+1}(B_1^\perp)\}\), where \(n = 1, 2, \ldots\) and \(\bar{n} = n - 1\) (\(\bar{n}\) begins from \(\bar{n} = 0\)). The effect caused by the inter-ribbon interactions on the envelope functions can be interpreted by the first order perturbation theory. Around \(k \cdot I_\perp = 0.5 \pi\), the matrix elements of \(h_{12}\) are proportional to \((\pi/2 - k \cdot I_\perp)\) because of \(\beta = 2 \cos(k \cdot I_\perp) \sim 2(\pi/2 - k \cdot I_\perp)\). Thus, the weak inter-ribbon interactions lift the degeneracy at \(k \cdot I_\perp = \pi/2\) and produce a two-level system, for example, \(n = 1\) and \(\bar{n} = 0\) subbands. The related envelope functions are \(\Psi(y, k \cdot I_\perp) = [\Psi_1(y, k \cdot I_\perp = \pi/2) - \Psi_2(y, k \cdot I_\perp = \pi/2)]/\sqrt{2}\), the bonding or antibonding of the envelope functions at \(k \cdot I_\perp = \pi/2\). As a result, the envelope functions of the \(n\) \((\bar{n})\) subbands chiefly distribute on the lower (upper) ribbon with the different spatial symmetries. In addition, inter-ribbon interactions have no influence on the envelope functions \(\Psi_{n=0}\) and \(\Psi_{n'=0}\).

The feature of the wave function at \(k \cdot I_\perp = 0.4 \pi\), as shown in Fig. 4(c), is dissimilar to that at \(k \cdot I_\perp = 0.499 \pi\) [Fig. 4(b)]. The charge carriers of the former distribute on two ribbon planes and each subenvelope function is of the same importance, whereas those of the latter concentrate only on one ribbon plane. The varying inter-ribbon interactions cause the redistribution of charge density. The definition of subband indices \(n\) and \(\bar{n}\) \((n'\) and \(\bar{n}'\)) is based on the spatial symmetry of the subenvelope function \(\psi_n(A_1^\perp)\). The subenvelope functions are proportional to the harmonic oscillator \(\phi_n\), for example, \(\psi_{n=1}(A_1^\perp) \sim \phi_1(A_1^\perp)\). The envelope functions of the \(n\) \((\bar{n})\) subbands are \(\{\phi_n(A_1^\perp), \phi_{n+1}(B_1^\perp), \phi_{n+1}(A_1^\perp), \phi_{n+1}(B_1^\perp)\}\) \((\{\phi_n(A_1^\perp), \phi_{n+1}(B_1^\perp), \phi_{n-1}(A_1^\perp), \phi_{n-1}(B_1^\perp)\}\) where the subband indices are \(n = 1, 2, \ldots, \bar{n} = n - 1\). The spatial symmetry \(n, n-1, n, n+1\) \((\bar{n}, \bar{n}-1, \bar{n}, \bar{n}+1\)\) is different from that \((n, n-1, n-1, n)\) at \(k \cdot I_\perp = 0\). The inter-ribbon interaction \(h_{12}\) plays the role as a rising operator, which changes \(\{\phi_{n-1}(A_1^\perp), \phi_{n+1}(B_1^\perp)\}\), the subenvelope functions at \(k \cdot I_\perp = 0\), to \(\{\phi_n(A_1^\perp), \phi_{n+1}(B_1^\perp)\}\). On the other hand, \(h_{12}(=h_{21})\), a lowering operator, changes \(\{\phi_n(A_1^\perp), \phi_{n-1}(B_1^\perp)\}\) to \(\{\phi_{n-1}(A_1^\perp), \phi_{n-1}(B_1^\perp)\}\), where \(\bar{n} = n - 1\). Due to the interactions between the \(n = \pm 2\) and \(\bar{n} = \pm 0\) subbands, the shape of \(\bar{n} = 0\) envelope functions is modified and its component \(\psi(B_1^\perp)\) almost disappears.

From \(k \cdot I_\perp = 0.4 \pi\) to \(k \cdot I_\perp = 0\), the gradually enhancing inter-ribbon interactions significantly modify the feature or the site amplitude of the \(n\) envelope functions [Fig. 4(d)]. At \(k \cdot I_\perp = 0\), the main feature of the envelope function \(\{\psi_n(A_1^\perp), \psi_{n+1}(B_1^\perp), \psi_{n+1}(A_1^\perp), \psi_{n+1}(B_1^\perp)\}\), as shown by heavy dots in Fig. 4(d), cannot simply be described by harmonic oscillator \(\phi_n\). Moreover, subenvelope functions \(\psi_{n=1}(B_1^\perp)\) and \(\psi_{n+1}(B_1^\perp)\) dominate the envelope function. As a result, \(\gamma_3\), the interaction between atoms \(B_1\) and \(B_2\), strongly affects the state energies and wave functions. For comparison, the subenvelope functions at \(k \cdot I_\perp = 0.3 \pi\) are shown by light dots in Fig. 4(d). The envelope function is an approximately linear superposition of components \(\phi_n(A_1^\perp), \phi_{n+1}(B_1^\perp), \phi_n(B_1^\perp), \) and \(\bar{n} = n - 1\) as shown by heavy dots \([\bar{n} = n - 1, n, n+1\] for comparison, the envelope functions \(\{\psi_{n=1}(A_1^\perp), \psi_{n+1}(B_1^\perp)\}\) are shown by light dots in Fig. 4(d). The envelope function is an approximately linear superposition of components \(\phi_n(A_1^\perp), \phi_{n+1}(B_1^\perp), \phi_n(B_1^\perp), \) and \(\bar{n} = n - 1\) as shown by heavy dots. Moreover, the envelope function \(\psi_{n-1}(B_1^\perp)\) and \(\psi_{n+1}(B_1^\perp)\) dominate the envelope function. As a result, \(\gamma_3\), the interaction between atoms \(B_1\) and \(B_2\), strongly affects the state energies and wave functions. For comparison, the envelope functions at \(k \cdot I_\perp = 0.3 \pi\) are shown by light dots in Fig. 4(d). The envelope function is an approximately linear superposition of components \(\phi_n(A_1^\perp), \phi_{n+1}(B_1^\perp), \phi_n(B_1^\perp), \) and \(\bar{n} = n - 1\) as shown by heavy dots.
\[
\Psi_n = \left[ 0, 0, \phi_n(A^2), \phi_{n-1}(B^2) \right], \quad n = n - 1, \quad k I z \sim \pi/2,
\]
\[
\Psi_n = \left[ \phi_n(A^1), \phi_{n-1}(B^1), \phi_n(A^2), \phi_{n+1}(B^2) \right], \quad n = 1,2,3, \ldots, \quad k I z \rightarrow 0,
\]
\[
\Psi_n = \left[ \phi_n(A^1), \phi_{n-1}(B^1), \phi_n(A^2), \phi_{n+1}(B^2) \right], \quad n = n - 1, \quad k I z \rightarrow 0.
\]

The characteristics of wave functions are applicable to the determination of optical transition channels. The optical absorption spectrum is
\[
A(\omega) \approx \sum_{\mu, \nu} \int_{\text{first BZ}} \frac{d k_x d k_z}{2 \pi 2 \pi} D(\omega) \times |M_{\mu, \nu}|^2,
\]
where \( \mu = n, \bar{n} \) and \( \nu = n', \bar{n}' \) are subband indices. \( D(\omega) \) is the joint density of states and \( |M_{\mu, \nu}|^2 \) is the velocity matrix element. According to the result of Ref. 32, the magnitude of the velocity matrix is \( |M_{\mu, \nu}| = |M_{\mu, \nu}^{\text{intra-ribbon}}| + |M_{\mu, \nu}^{\text{inter-ribbon}}| \), where \( |M_{\mu, \nu}|^{\text{inter-ribbon}} \) is proportional to \( \langle \Psi_\mu(k, l) | \Psi_{\nu}(k, l) \rangle \) of the initial state \( \langle \Psi_\mu(k, l) | \Psi_{\nu}(k, l) \rangle \) of the final state. The interribbon projection (inter-ribbon) denotes the initial and final states located at the same (different) ribbons. The interribbon projection, for example, is
\[
\langle \Psi_n(k, l) | \Psi_n'(k, l) \rangle_{\text{intra-ribbon}} = \langle \psi_n(A^1) | \psi_n'(B^1) \rangle + \langle \psi_n(A^2) | \psi_n'(B^2) \rangle + \langle \psi_n(B^1) | \psi_n'(A^1) \rangle + \langle \psi_n(B^2) | \psi_n'(A^2) \rangle.
\]

The velocity matrix element \( M_{\mu, \nu} \) depends on the spatial symmetries of the initial and final states, and thus determines the selection rule and the effective transition channels. At \( k I z = \pi/2 \), only the interribbon optical transition, \( |M_{\mu, \nu}^{\text{intra-ribbon}}| \) makes contribution to the velocity matrix element \( |M_{\mu, \nu}| \). There is only one group of subbands, i.e., \( \mu = n \) and \( \nu = n' \). Therefore, the optical selection rule is predicted to be \( \delta_{n-n'} = \pm 1 \), where \( n = 0, 1, 2, 3, \ldots \) and \( n' = 0, 1, 2, 3, \ldots \). The selection rule is the same as that of a monolayer graphene ribbon.19

Away from \( k I z = \pi/2 \), there are four possible optical transition channels \( n' \rightarrow n, n' \rightarrow \bar{n}, \bar{n}' \rightarrow n, \) and \( n' \rightarrow \bar{n} \) [Fig. 5(b)]. According to the spatial symmetry of envelope functions [Eqs. (7d) and (7e)], the corresponding selection rules of the four transitions are predicted to be \( \delta_{n-n'} = \pm 1 \), \( \delta_{n-n'} = \pm 1 \), and \( \delta_{\bar{n}-n} = \pm 1 \). The change in the state energies caused by interribbon interactions might alter the peak positions of joint density of states, and the modification of the shape and site amplitude of envelope functions might give rise to the vivid variation of the magnitude of velocity matrix element \( M_{\mu, \nu} \). Thus, the optical spectra of the Bernal ribbons are expected to be more complicated in peak number, peak position, and peak height than those of a monolayer or bilayer ribbon. The work to calculate the optical spectra of the Bernal ribbon is ongoing.

IV. CONCLUSIONS

The Peierls coupling tight-binding method is employed to investigate the anisotropic magneto-electronic structures of multilayer graphene ribbons. They are strongly dependent on the B-field strength and the inter-ribbon interactions. \( B \) can induce Landau levels along \( k_x \) and change energy spacing. The inter-ribbon interactions significantly affect state degeneracy, energy dispersions, and Landau plot. They destroy the symmetry of magnetoband structures. They also produce concave and convex subbands along \( k_x \). The magnetoband structures are strongly anisotropic. There are many doubly degenerate Landau levels and singlet 1D curving bands along the \( k_x \) and \( k_z \) directions. Moreover, the \( k_x \)-dependent inter-ribbon interactions modify the shape of wave functions, alter the spatial symmetry, and arouse the change in charge-carrier distribution. The findings are further used to predict the optical selection rule. Most importantly, the large Bernal graphene ribbons are expected to be almost identical to the bulk graphite in low-energy magneto-electronic properties. Our work is useful in understanding the bulk graphite, e.g., magneto-electronic excitations and magneto-optical absorption spectra. The predicted magneto-electronic properties could be examined by transport and optical measurements.

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