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Interaction between the intrinsic edge state and the helical boundary state of topological insulator phase in bilayer graphene

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ABSTRACT

Graphene has intrinsic edge states localized at zigzag edge or lattice defect. Helical boundary states can also be established in such a two-dimensional carbon material at the boundary of topological insulator (TI) phase realized by the extrinsic Rashba spin–orbital coupling (SOC) in gated bilayer graphene. We theoretically investigate the interaction between these two kinds of edge (boundary) states when they coexist in a bilayer graphene. We find that this interaction gives rise to some very interesting results. In a zigzag edged nanoribbon of bilayer graphene, it is possible that the TI helical state does not localize at the TI phase boundary. Instead it moves to the nanoribbon edge even though the SOC is absent therein. In a bulk lattice of bilayer graphene embedded with two line defects, the numbers of helical state subbands at the two line defects are not equal to each other. In such a case, the backscattering lacking is still forbidden since the Kramers pairs are valley polarized.

1. Introduction

Edge states play the key roles in explaining many important electronic transport properties in two-dimensional (2D) electron systems. For instance, the quantum Hall edge states carry the current flow to give rise to the perfect Hall conductance plateaux. Another typical example of edge state is the so-called helical states at an edge of a 2D topological insulator [1,2]. In such states electrons with opposite spins counterpropagate in a given edge. Just due to such a helicity of the edge state, a 2D TI is expected to exhibit the quantum spin Hall effect.

Shortly after the first experimental acquirement of a graphene sample [3], it was observed that bilayer graphene also exhibits remarkable phenomena [4,5]. In bilayer graphene the bands around the Dirac Points are parabolic dispersion relationship, and its bandgap can be opened and tuned via a chemical doping [6] or externally by applying a gate voltage [7,8]. In spite of the first-principle calculations shows weak SOC in bilayer graphene [9,10], some theoretical studies proposed that bilayer graphene can be driven into 2D TI state by gating the bilayer graphene to induce a strong extrinsic SOC [11,12]. As a result, the helical state can be realized in a controllable way in bilayer graphene at the boundary of TI phase.

As an unusual electronic material, graphene possesses a special kind of edge states which does nothing with the magnetic field or SOC. Such an edge state always adheres to a zigzag edge [13–15] or lattice defects [16] even in an ordinary graphene lattice. Similarly to the helicity of the TI edge state, this intrinsic edge state of graphene is valley filtered in the sense that electrons counterpropagate if they have the opposite valley degrees of freedom. Moreover, in a gated bilayer graphene such an edge state persists in the bulk bandgap as a gapless mode [11], bearing an analogy with the TI edge state. Due to the topological proximity effect [17], the topological graphene nanoribbon heterostructure becomes an expanded TI. It can be predicted that such an interesting phenomenon could arise when the valley filtered edge state and the TI helical state coexist in bilayer graphene.

To address this issue, in the present work we firstly consider a zigzag edged nanoribbon of bilayer graphene in which a partial strip region is assumed in the TI phase driven by a Rashba SOC. We find that as the TI phase boundary gets close to the zigzag edge of the nanoribbon, the TI helical state becomes to localize at the nanoribbon edge, rather than the TI boundary, though no SOC appears around the nanoribbon edge. Meanwhile, if we introduce a pair of line defects to the bulk lattice of bilayer graphene to induce the valley filtered edge state, instead of the zigzag edges, the numbers of gapless modes (helical state bands) localized at the opposite boundaries are not equal to each other. There are three pairs and one pair of gapless modes at the left and right boundaries, respectively. Besides, these helical state subbands are still

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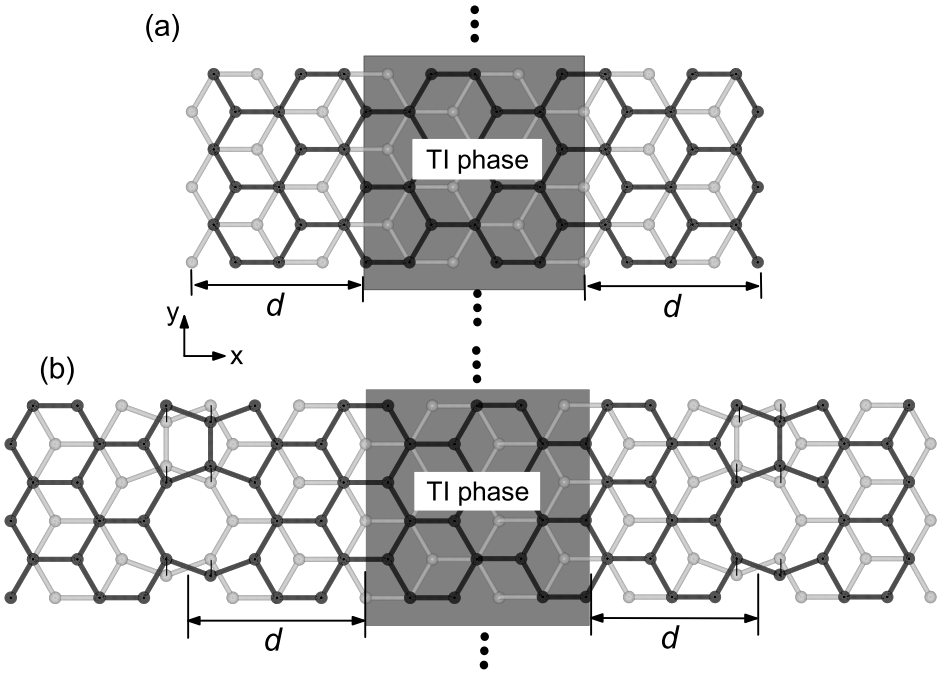

Fig. 1. Lattice structures of (a) a zigzag edged nanoribbon of bilayer graphene; (b) a bilayer graphene embedded with two parallel line defects. The thin lines connecting the nearest-neighbor inter-layer atomic pairs around the line defect indicate the nonzero tight-binding inter-layer hopping energy between these atoms. The shaded strip stands for the TI phase driven by the nonzero SOC. d labels the strip width from the TI boundary to the zigzag edge or the line defect.

valley filtered in the vicinity of each valley inside bandgap. Thus, the backscattering lacking is still forbidden since the Kramers pairs are valley polarized.

2. Structure and Hamiltonian

In the present work, we consider two graphene structures to investigate the interaction between the different kinds of edge states. The first one is a zigzag edged nanoribbon of bilayer graphene (ZENR-BG) whose lattice is depicted in Fig. 1(a). In such a nanoribbon the Rashba SOC is restricted within the partial region shown as the shaded strip in Fig. 1(a). A sufficiently strong Rashba SOC can drive this strip into TI phase. Hence the helical states are induced at the two opposite boundaries of the TI phase, which coexist with the graphene intrinsic edge states localized at the zigzag edges of the ZENR-BG. The other structure under our consideration is a bulk bilayer graphene lattice embedded with a pair of parallel line defects, see Fig. 1(b). Hereafter we abbreviated such a structure to LD-BG. From Fig. 1(b) we can see that in the lattice of a LD-BG, each line defect along y direction consists of the periodic repetition of a pair of pentagonal rings plus an octagonal ring in each layer. In a LD-BG structure the line defects play a similar role as the zigzag edges in a ZENR-BG to induce the valley filtered edge (boundary) states. In a monolayer graphene, such a line defect upto a millimeter scale has been experimentally observed as the boundary of graphene single-crystalline domains [18]. Besides, it is thus far experimentally feasible to control the orientation and size of a line defect in graphene lattice [19]. Therefore, it is a reasonable anticipation that the line defect can be formed in an epitaxially grown bilayer graphene lattice.

We employ the tight-binding model to study the edge (boundary) state properties of these two structures. The π electronic tight-binding Hamiltonian of them can be written in a unified form. It reads

$$\mathcal{H} = \mathcal{H}_T + \mathcal{H}_B + \mathcal{H}_i \tag{1}$$

where $\mathcal{H}_{T(B)}$ denotes the intra-layer interaction in the top (bottom) layer; and $\mathcal{H}_i$ includes the inter-layer interaction and the gating potential. Within the nearest-neighbor approximation we can further write out

$$\mathcal{H}_{T(B)} = -t \sum_{\langle ij\rangle\alpha} c^{\dagger}_{i\alpha} c_{j\alpha} + \mathrm{i}t_R \sum_{\langle ij\rangle\alpha\beta} (\mathbf{s}_{\alpha\beta} \times \mathbf{d}_{ij})_z c^{\dagger}_{i\alpha} c_{j\beta} \tag{2}$$

here, the first term is the usual intra-layer hopping term. The operator $c_{i\alpha}$ ($c^{\dagger}_{i\alpha}$) annihilates (creates) an electron with the spin $\alpha = \pm 1$ on site i; $\langle ij\rangle$ stands for that the summation only runs over the nearest-neighbor intra-layer atomic pair. And t is the corresponding hopping energy. As a simplest approximation, it is assumed to take a uniform value, i.e., $t \simeq 2.8$ eV, no matter whether the involved atomic pair is in the ordinary hexagonal ring or the pentagonal and octagonal rings around the line defects. The second term at the righthand side of Eq. (2) is the Rashba SOC with the coupling strength t_R. As mentioned above, only in the shaded strip region t_R takes a nonzero value. $\mathbf{s}$ are the electronic spin Pauli matrices, and $\mathbf{d}_{ij}$ is the lattice vector pointing from site j to site i.

The last term in Hamiltonian (1) is given by

$$\mathcal{H}_i = U \sum_{i\in T,\alpha} c^{\dagger}_{i\alpha} c_{i\alpha} - U \sum_{i\in B,\alpha} c^{\dagger}_{i\alpha} c_{i\alpha} - t_{\perp} \sum_{i\in T, j\in B,\alpha} (c^{\dagger}_{i\alpha} c_{j\alpha} + c^{\dagger}_{j\alpha} c_{i\alpha}) \tag{3}$$

where $\pm U$ stands for the onsite energies of the top and bottom layers controlled by a gate voltage. $t_{\perp}$ ($\simeq 0.4$ eV) is the hopping energy between the nearest-neighbor inter-layer atomic pair. At the ordinary hexagonal lattice points, such an atomic pair refers to the two carbon atoms exactly aligned with each other in the normal direction of the lattice plane. Around the line defects, the nearest-neighbor inter-layer atomic pair is labeled by a thin line in Fig. 1(b).

3. Results and discussions

With the tight-binding Hamiltonian we can calculate the band structure of both the ZENR-BG and LD-BG structures introduced