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Topological states in two-dimensional hexagon lattice bilayers

Ming-Ming Zhang, Lei Xu, Jun Zhang *

School of Physics Science and Technology, Xinjiang University, Urumqi 830046, China

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ABSTRACT

We investigate the topological states of the two-dimensional hexagon lattice bilayer. The system exhibits a quantum valley Hall (QVH) state when the interlayer interaction $t_\perp$ is smaller than the nearest neighbor hopping energy t, and then translates to a trivial band insulator state when $t_\perp/t > 1$. Interestingly, the system is found to be a single-edge QVH state with $t_\perp/t = 1$. The topological phase transition also can be presented via changing bias voltage and sublattice potential in the system. The QVH states have different edge modes carrying valley current but no net charge current. The bias voltage and external electric field can be tuned easily in experiments, so the present results will provide potential application in valleytronics based on the two-dimensional hexagon lattice.

1. Introduction

The two-dimensional hexagon lattice has become one of the most important topics in condensed physics and material science [1–3], since the successful fabrication of graphene [4]. Recently, many new materials of graphene family have been synthesized, such as silicene, hafnene, germanene and stanene [5–9], which have a monolayer hexagon structure, and their energy spectra contain Dirac cones. In field theories, Dirac particles and associated gauge fields have been intensively investigated from a topological point of view, so electronic properties for the hexagon lattice may open new avenues for condensed matter phenomena [10,11]. This is a class of materials that possibly hold both topological and superconducting properties. The electronic properties of topological insulators (TI) and the two-dimensional hexagon lattice have been extensively studied in recent years [12–15], owing to their unusual structures and remarkable potential in advanced nanoelectronics applications.

For the material of graphene family, the low energy dispersion is linear around two valleys at K and K' points of the Brillouin zone (BZ). The two valleys are degenerate in energy and related by the time reversal symmetry [16–20]. The independence and degeneracy of the valley degree of freedom suggest that it may be used to control an electronic device [21], in the same way as electron spin used in spintronics or quantum computing. The valley electronic has become one of hotspots of condensed matter. A very important issue in valleytronics is how to generate pure valley current, which consists of two identical currents flowing in opposite directions in the two valleys, resembling the pure spin current in spintronics. In two-dimensional system, it was proposed that full valley filters could be realized in nanojunctions such as wedge-shaped graphene nanoribbons [22], and graphene junctions [18], as well as graphene sheet with grain boundaries [23].

In the research of two-dimensional hexagon lattice, bilayer systems have attracted a lot of attention [24–30]. The various interlayer interaction between the nearest neighbor of the two layers makes the bilayers possess different properties [31]. The changing of the interlayer interaction also can shift the position of Dirac points. Due to the atoms of a slice of bilayer system composed of sp^2 hybridization, each layer of the system has a flat hexagon structure [32,33]. However, when the sp^2/sp^3 mixed hybridization is employed in the bilayer system, the most stable configuration prefers to occur as low-buckled structure, such as silicene, as shown in Fig. 1(b) [7,34]. Compared with monolayer system, the extra layer degree of freedom can lead to many new physical phenomenons, and it is also easier to be controlled in experiments [24–26]. Besides, in terms of topological properties, bilayer is different from single layer. A quintessential example should be cited that the bilayer system formed by the combination of two layers of quantum spin Hall insulator becomes a trivial band insulator (BI) [35], but when a bias voltage is introduced, the bilayer system goes over to topologically nontrivial. This indicates that the topological properties of bilayer are quite different from the single [24]. To obtain more concerning two-dimensional hexagon lattice bilayers, by analyzing the changing of Dirac points and topological quantum numbers, we investigate the quantum valley Hall (QVH) state of two-dimensional hexagon lattice bilayers.

In this paper, we present a study of the QVH state and single-edge QVH state of the gated two-dimensional hexagon lattice

* Corresponding author.
E-mail address: zhj@xju.edu.cn (J. Zhang).

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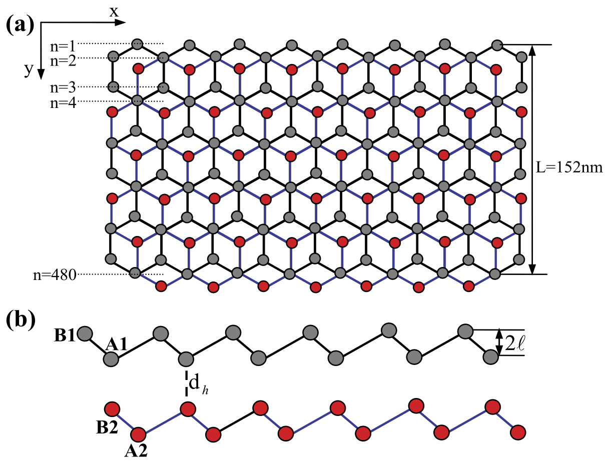

Fig. 1. (a) Schematic of a zigzag edged nanoribbon of hexagon lattice bilayer. (b) Side view of the bilayer lattice.

bilayer with various interlayer interaction. By investigating the band structure, especially the gap of edge band, Chern number, valley Chern number and edge modes, we show that the gated bilayer system exhibits a QVH state, single-edge QVH state and BI state respectively, depending on the parameter $t_{\perp}/t$. For a given bilayer system with fixed interlayer interaction $t_{\perp}$, these topological phase transitions from QVH phase to single-edge QVH phase, and from single-edge QVH phase to BI can be tuned by changing bias voltage and sublattice potential. In particular, we find that these phase transitions occur without even bulk gap closing, and the single-edge QVH is easy to implement valley current without any accompany of charge current.

2. The model and method

The tight-binding Hamiltonian of the monolayer hexagon lattice including sublattice potential can be written as [36]

$$H_{MLS} = -t \sum_{\langle ij\rangle\alpha} C^{\dagger}_{i\alpha} C_{j\alpha} - \ell \sum_{i\alpha} \mu_i E_z C^{\dagger}_{i\alpha} C_{i\alpha}, \tag{1}$$

here $C^{\dagger}_{i\alpha}(C_{i\alpha})$ is a creation (annihilation) operator for an electron with spin α on site i. The first term describes the nearest neighbor hopping with hopping energy t. The second term represents a staggered sublattice potential with E_z describing the uniform electric field applied to the sheet, $2\ell = 0.46$ Å describing the space between A and B sites, and $\mu_i = +1(-1)$ for the $A(B)$ site. Due to the bulked structure, a sublattice potential is induced by an external out-of-plan electric field.

The Hamiltonian of AB-stacked bilayer system in the presence of sublattice potential and antisymmetric interlayer bias voltage can be written as [25,26]

$$H_{BLS} = H^{T}_{MLS} + H^{B}_{MLS} + t_{\perp} \sum_{i\in T, j\in B,\alpha} (C^{\dagger}_{i\alpha} C_{j\alpha} + C^{\dagger}_{j\alpha} C_{i\alpha}) + U \sum_{i\in T,\alpha} C^{\dagger}_{i\alpha} C_{i\alpha} - U \sum_{j\in B,\alpha} C^{\dagger}_{j\alpha} C_{j\alpha}, \tag{2}$$

with $H^{T,B}_{MLS}$ for the top (T) and bottom (B) monolayer Hamiltonian. Interlayer interaction between the nearest neighbor of the two layers is given by the third term with an interaction energy $t_{\perp}$. The interlayer potential difference $2U$ is given by the last two terms. Thus, the spatial inversion symmetry of the two-dimensional hexagon lattice bilayer is broken by the interlayer potential.

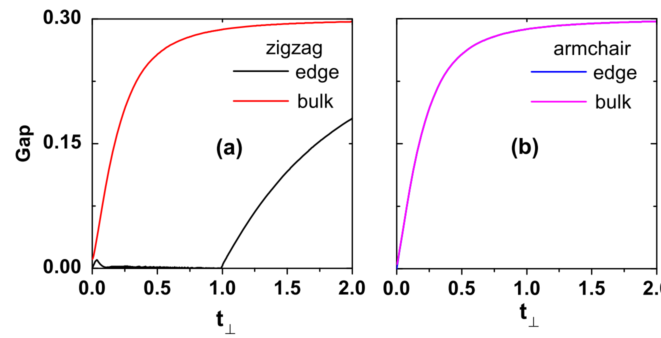

Fig. 2. The gap of bulk band and edge band as a function of interlayer interaction $t_{\perp}$ for bilayer hexagon lattice with (a) zigzag and (b) armchair terminations. The results are obtained with sublattice potential $\triangle = 0$ and interlayer potential $U = 0.15t$.

The topological insulator states of bilayer system can be classified by Chern number $\mathcal{C}$ and valley Chern number $\mathcal{C}_v$ [37–39], which can be given by

$$\mathcal{C} = \mathcal{C}^{K} + \mathcal{C}^{K'} \tag{3}$$

$$\mathcal{C}_v = \mathcal{C}^{K} - \mathcal{C}^{K'} \tag{4}$$

The valley Chern number can be calculated from [40,41]

$$\mathcal{C}^{\eta} = \frac{1}{2\pi} \sum_{n} \int dk_x dk_y (\Omega_n(\mathbf{k}))^{\eta}, \tag{5}$$

where $\eta = \pm 1$ is the valley index, the integral around the K (K') point in the Brillouin zone, and Ω_n is the momentum-space Berry curvature for the nth band [38,39,42,43]

$$\Omega_n(\mathbf{k}) = -\sum_{n'\neq n} \frac{2\mathrm{Im}\langle\psi_{nk}|v_x|\psi_{n'k}\rangle\langle\psi_{n'k}|v_y|\psi_{nk}\rangle}{(\varepsilon_{n'} - \varepsilon_n)^2}. \tag{6}$$

The summation in momentum space is over all occupied bands below the bulk gap and $v_{x,y} = \partial H/\partial k_{x,y}$ is the velocity operator. Therefore, we can classify the topological quantum states by calculating the above topological quantum numbers in the vicinity of valley K and K' [37,40].

3. Results and discussions

Two-dimensional hexagon lattice bilayers have been experimentally observed to be AA or AB stacked configuration. Under the bias voltage, a band gap can open in AB-stacked bilayer system but still close in AA-stacked bilayer system [14], thus we only focus on AB-stacked bilayer system. Two-dimensional hexagon lattice ribbon have two principal edge terminations along and perpendicular to the band-length direction, respectively, known as armchair and zigzag terminations [32]. We first examine the energy spectra of the AB-stacked bilayer ribbon with both zigzag termination and armchair termination. The width of the zigzag edged nanoribbon of hexagon lattice bilayer is L = 152 nm (containing 240 zigzag chains) in this paper, as shown in Fig. 1(a).

For two-dimensional hexagon bilayers, the interlayer interaction can be tuned by an pressure [44], so we firstly show the evolution of gaps of bulk and edge bands of bilayer ribbon with zigzag termination in Fig. 2(a). We find the gap of bulk band opens all the time. However, the gap of edge band closes for $t_{\perp}/t < 1$, but the gapless edge states disappear when $t_{\perp}/t > 1$.[1] And we find that $t_{\perp}/t = 1$ is the critical situation. Unfortunately, for two-dimensional hexagon bilayer with armchair termination, the gaps of both bulk and edge

[1] When $t_{\perp}$ is very close to zero, there is a very small edge gap [see the little peak in Fig. 2(a)] due to the effect of interlayer potential ($U = 0.15t$).