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Topological state engineering by in-plane electric field in graphene nanoribbon

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ABSTRACT

We investigate the electronic states of a zigzag graphene nanoribbon in the presence of mutually perpendicular electric and magnetic fields. We find that both edge and bulk states are localized in the vicinity of zero energy, leading to spin-polarized states and quantized transport in the system. A quantum spin Hall phase is characterized by helical edge and tilted bulk states. By tuning Fermi energy and in-plane electric field, a topological phase transition is also realized. The electronic states support the transport of spin and charge, and the corresponding spin and charge Hall conductivities are calculated in a four-terminal geometry.

1. Introduction

The processing of graphite has made the isolation of two-dimensional graphene sheets [1]. This system has been studied theoretically and implied nanoelectronic devices [2–5]. The material is unique because the underlying honeycomb lattice has a band structure with Dirac points at the corners of the Brillouin zone, in which there are two inequivalent Dirac points. In this low-energy region, the system can be described by the Dirac equation.

Under a perpendicular magnetic field, the Landau levels (LLs) of graphene are spaced unevenly due to the chiral nature of carriers, giving rise to quantum Hall (QH) effect [6–8]. The quantized Hall conductivity is $\sigma_{xy} = \nu_1 e^2/h$ among filling factors $\nu_1 = \pm 4(n+1/2)$, where h is Planck's constant, e is electron charge, n is an integer and the factor 4 is resulted from spin and valley degeneracy [2,6,7,9]. The existence of the quantum spin Hall (QSH) effect [10–12] was first proposed in a graphene film, in which the spin–orbit interaction opened a small band gap [13]. Soon afterwards, a quantized longitudinal resistance platform was observed owing to the QSH effect which was triumphantly achieved in CdTe/HgTe quantum wells [14].

The zigzag graphene nanoribbon is known to have flat bands connecting two valleys, corresponding to the localized edge states [15–17]. It is found that a bulk energy gap is opened in zigzag-edged half-infinite graphene [18,19]. Recently, graphene nanoribbon in the presence of crossed uniform electric and magnetic fields is shown to exhibit dramatic changes in band structure [20] and transport properties [21]. Lukose et al. [20] found a tilted LL of graphene when the ratio of electric field to magnetic field exceeds a certain critical value, which is different from the LLs of two-dimensional electron gas. Subsequently, the properties of a graphene nanoribbon [22] in both in-plane electric bias and perpendicular magnetic field are investigated. It exhibited tunable shortcut edge states yielding some interesting transport effects. Moreover, the even symmetry of the energy band in armchair graphene nanoribbon preserves with each of the electric and magnetic fields applied. However, when the two fields are applied together, they break both the time reversal symmetry and the inversion symmetry and reverse the dispersion parity, resulting in the mixture of the electron and hole subbands near the zero energy [21].

In this paper, we study the electronic states caused by the tilted LLs of zigzag graphene nanoribbon under mutually perpendicular electric and magnetic fields [Fig. 1]. The states in the vicinity of zero energy are localized and can give rise to a QSH state which belongs to both edge and tilted bulk states. A topological phase transition is shown by changing Fermi energy or the in-plane electric field. The spin current is also generated in a four-terminal geometry.

2. Models and methods

We begin with the monolayer graphene nanoribbon subjected to a perpendicular magnetic field $\mathbf{B} = (0, 0, -B)$ and an in-plane uniform electric field ε. The Hamiltonian of this tight-binding model can be written as

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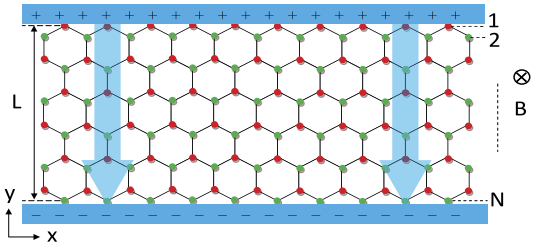

Fig. 1. Schematic of a zigzag graphene nanoribbon along x axis threaded by an in-plane uniform electric field ε and perpendicular magnetic field **B**. The direction of the in-plane field is indicated by the blue arrows. The width of nanoribbon is $L = (3N/4 - 1)a = 21.2$ nm with $N = 200$ and $a = 0.142$ nm. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$$H = -t \sum_{<i,j>,\sigma} e^{i\phi_{ij}}(C^{\dagger}_{i,\sigma}C_{j,\sigma} + H.c.) + M\sum_{i,\sigma}\sigma_z C^{\dagger}_{i,\sigma}C_{i,\sigma} + \sum_{i,\sigma}\epsilon_i C^{\dagger}_{i,\sigma}C_{i,\sigma}. \quad (1)$$

The first term in Hamiltonian describes the nearest-neighbor hopping with t being the amplitude of the hopping energy and $C^{\dagger}_{i,\sigma}$ ($C_{i,\sigma}$) being the electron creation (annihilation) operator on site i with spin index σ and ϕ_{ij} being the magnetic flux. Because electron hopping is from site j to site i, there comes $\phi_{ij} = \int_j^i \mathbf{A}\cdot\mathbf{dr}/\phi_0$ with the Landau gauge $\mathbf{A} = (0, -Bx, 0)$ and $\phi_0 = \hbar/e$. The second term corresponds to the Zeeman splitting with strength M, in which σ_z is the Pauli spin matrix. The third term represents the in-plane electric field ε along the y direction with on-site energy ϵ_i. The on-site energy is $\epsilon_i = eU[1 - 3a(i-1)/2L]/2$ for $i = 1, 3, ..., N-1$ and $\epsilon_i = eU[1-(3i-4)a/2L]/2$ for $i = 2, 4, ..., N$, where U is the electric bias, a is the lattice constant and L is the width of ribbon.

In order to explore transport properties, we use the Lattice Green's function method [23,24] to compute the two-terminal conductance. In the tight-binding system, the transmission coefficient from terminals q to p is given by $T_{pq} = \mathrm{Tr}[\Gamma_p G_{pq}\Gamma_q G^{\dagger}_{pq}]$, where $\Gamma_p(E) = i(\Sigma_p - \Sigma^{\dagger}_p)$ is the broadening function of terminal p and the self-energy Σ_p is related to elements of the Green's function between sites at the surface of the terminal. $G_{pq}(E) = [E - H_D - \Sigma_L(E) - \Sigma_R(E)]^{-1}$ is the Green function containing sites in the central device that connects to terminals p and q.

3. Results and discussions

In our numerical calculations, the energy spectrum is obtained by directly diagonalizing the Hamiltonian equation (1) with the consideration that all energies and lengths are expressed in units of the hopping energy t ($t = 2.71$ eV) and the lattice constant a ($a = 0.142$ nm), respectively. The system enters the Landau quantization regime only if the nanoribbon width L is much larger than the magnetic length [25] $l_B = \sqrt{\hbar/eB}$, i.e. $L \gg l_B$, where B is the magnetic field. The calculated energy spectra for different widths and different magnetic fields show that the eigenvalues are scaling functions of B and L. These scaling functions suggest that the same behavior of the energy spectrum be expected at small size but a large magnetic field. Therefore, we only consider a smaller system and external fields even higher than available in experiments. Hereafter, the width of graphene nanoribbon is denoted by $L = (3N/4 - 1)a = 21.2$ nm $\approx 10l_B$, where $N = 200$ denotes the total number of atomic sites in the y direction of the graphene nanoribbon, and the magnetic flux is $\phi = 0.002$.

It was proved analytically that in the low-energy range of graphene spectrum, the spacing scales among LLs decrease in both

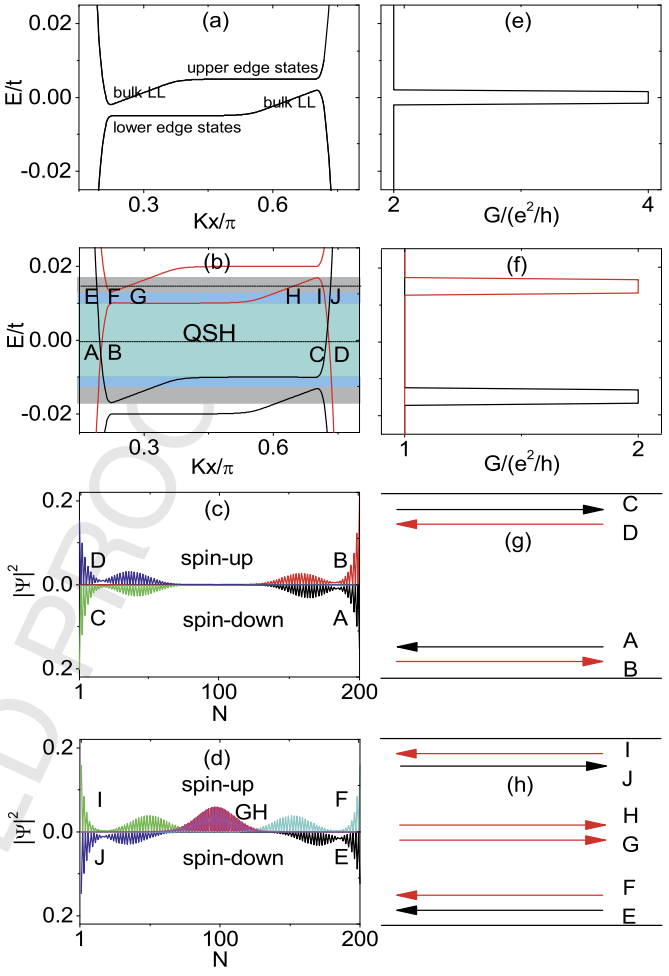

Fig. 2. (a) and (b): Energy dispersion of zigzag-edged graphene nanoribbon at fixed magnetic flux $\phi = 0.002$ and fixed electric bias $U = 0.01$ for (a) $M = 0$ and (b) $M = 0.015$. The red and black lines denote bands of spin-up and spin-down states. The part of inclined lines are labeled "bulk LL" and parallel lines are labeled "edge states". (c) and (d): The probability density distributions of electronic states intersected by dashed lines in energy spectrum. (e) and (f): Two-terminal conductances corresponding to (a) and (b). (g) and (h): Schematic propagations of conducting channels labeled by the letters in (b). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

conduction and valence bands as the electric field increases [20], and all LLs incline for a critical value of the ratio $\beta = \varepsilon/v_F B = SU/(ev_F L\phi)$ ($\phi = BS$, $S = 3\sqrt{3}a^2/2$, $U = e\varepsilon L$) of the electric filed to magnetic field. The titled levels exist when the value β is smaller than an unity by the tight-binding calculation [22].

Applying an in-plane electric and a perpendicular magnetic fields on the zigzag graphene nanoribbon, the energy spectrum distortion destroys the electron–hole symmetry and time-reversal symmetry but the odd symmetry $E_{h,k} = -E_{e,-k}$ (h, e and k represent hole, electron and wave vector respectively) of the energy spectrum are retained [21] as illustrated in Fig. 2(a). We find that the tilted LLs are twice degenerate due to the spin degeneracy and the corresponding two-terminal conductance is $G = 2ne^2/h$ ($n = 1, 2, 3, \cdots$) at a fixed electric bias $U = 0.01$ (corresponding to $\varepsilon = 1.3 \times 10^6$ V/m and $\beta = 0.01$) without the Zeeman splitting.

When the Zeeman splitting is taken into account, the Fermi energy is within the gap $E_F < |M - U/2|$ and intersect four energy bands labeled by letters A–D in Fig. 2(b). The electron probability densities and flowing directions of the four representative states are shown in Figs. 2(c) and 2(g). The edge modes labeled A and B are located on the lower boundary, and the others are located on the upper boundary. Furthermore, they are helical states formed by