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Quantized transport of interface and edge states in bent graphene

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ABSTRACT

We explore the transport behavior of interface and edge states in bent graphene under a magnetic field. The bending angle can change the distribution of interface and edge states, resulting in an interesting evolution of quantized conductance. The interface state vanishes when the bending angle is not less than $\pi/2$, whereas the edge state remains. In the presence of Zeeman splitting, the transport properties are also considered and a quantum spin Hall effect is found. These results may provide a way to control the interface current.

1. Introduction

Graphene has attracted great attention since it was successfully fabricated in experiment. It is the first truly two-dimensional material and has many unconventional properties [1,2], such as the linear dispersion [3,4] and quantum Hall effect [5,6]. Due to the linear dispersion near zero energy, the quantum Hall effect in graphene is characterized by chiral edge states and the quantized conductance is given by $\sigma_{xy} = 4(n+1/2)e^2/h$ with n being an integer [5]. However, the quantum spin Hall (QSH) effect, which is characterized by helical edge states, is also predicted in graphene [7,8] and was later experimentally realized in HgTe/CdTe quantum well [9,10]. These helical edge states are fully spin-polarized formed by counter propagating edge states with opposite spins and are preserved by time-reversal symmetry [7,8]. Moreover, electron transport properties of graphene have been extensively studied in electric and magnetic fields [1,2], and some interesting results have been obtained, such as particular transport properties in graphene with multiple magnetic barriers [11,12] and tunable controllable electronic states in graphene by both electric and magnetic fields [13].

Two-dimensional graphene can be bent into the third dimension without degradation to its structural properties and electron transport [14–16]. Therefore, the bent graphene has also been a focus of intense interest. The bend effectively produces a new type of Hall edge state along the bent region [17–19], leading to some novel transport properties in bent graphene [20–22]. The effect of bending curvature has been studied in bent graphene [18,23]. The tight-binding approximation in planar graphene only considers the π and π^* bands due to the hopping between p_z orbitals perpendicular to graphene plane. However, there is a curvature-induced misalignment of the p_z orbitals in bent graphene. Thus, the hopping integral should be modified as $t_0 = t\cos\alpha$ (α is the misalignment angle between p_z orbitals) [18].

This provides a train of thought for us to study the transport properties of bent graphene. In this work, we consider the bent graphene ribbon depicted schematically in Fig. 1(a). It consists of a graphene ribbon with a zigzag edge bent along the x direction. The graphene ribbon is bent into a wedge shape, as shown in Fig. 1(c). The bending angle θ between two planar regions is an arbitrary value. The bent graphene ribbon is divided into three regions, top planar region (TR), bottom planar region (BR) and middle bent region (MR). The magnetic field $\vec{B}$ is in the z direction and perpendicular to the BR of bent graphene, as shown in Fig. 1(c). We study the effect of bending angle to interface states, edge states and quantized conductances in a magnetic field. By changing of the bending angle, different interface and edge states are found in the bent graphene ribbon. Besides, the effect of curvature-modified hopping integral and width of the MR is also considered. The results show that they hardly affect the spatial distributions of interface and edge states. Finally, we discuss the electron transport property in the presence of Zeeman splitting and find that the system can host a QSH phase.

2. Model and method

In a perpendicular magnetic field $\vec{B} = (0, 0, B_z(x))$, the Hamiltonian of tight-binding model takes the form

$$H = -t\sum_{\langle ij\rangle}(e^{i\phi_{ij}}c_i^\dagger c_j + \text{h.c.}), \tag{1}$$

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where t is the nearest-neighbor hopping integral on the honeycomb lattice and ϕ is the gauge potential for the nonuniform magnetic field. The operator $c_i^\dagger$ (c_i) creates (annihilates) an electron at site i, and $\langle ij \rangle$ denotes nearest-neighbor sites.

In terms of the Landauer–Büttiker formula, the conductance with spin σ can be calculated by the equation $G_\sigma = T_\sigma e^2/h$ [24–26]. The transmission coefficient T_σ from lead r to lead l with spin σ is described by

$$T_\sigma = \mathrm{Tr}[\Gamma_{l\sigma} G_\sigma^R \Gamma_{r\sigma} G_\sigma^A], \tag{2}$$

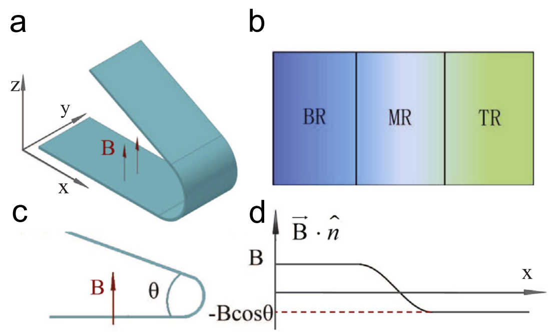

Fig. 1. (a) A zigzag-edge graphene ribbon is bent along the x direction. The uniform magnetic field $\vec{B}$ is perpendicular to the bent graphene ribbon. (b) A topological equivalent geometry obtained by unbent graphene ribbon. TR, BR and MR correspond to top planar region, bottom planar region and middle bent region respectively in (a). L_x represents the width of the MR. (c) The plane projection of (a) and θ is the bending angle. (d) The profile of the effective magnetic field in an equivalent unbent graphene ribbon.

where $\Gamma_{\ell\sigma} = i[\Sigma_{\ell\sigma}^R - \Sigma_{\ell\sigma}^A]$ is the coupling between conductor and lead ℓ ($\ell = l, r$) with $\Sigma_{\ell\sigma}^{R/A}$ being the self-energy. The retarded Green's function of the sample G_σ^R has a form $G_\sigma^R = [G_\sigma^A]^\dagger = [E - H_\sigma^c - \Sigma_{l\sigma}^R - \Sigma_{r\sigma}^R]^{-1}$, where H_σ^c is the Hamiltonian of the conductor region.

3. Results and discussion

In Fig. 1(a), we show the bent graphene ribbon under a uniform magnetic field. The system can be described by a topological equivalent geometry suffering an effective magnetic field shown in Fig. 1(b) and (d). The magnetic field $\vec{B}$ is perpendicular to BR, whereas the field is $-B\cos\theta$ [θ is the bending angle shown in Fig. 1(c)] in TR. In MR, the effective magnetic field is the normal component of magnetic field, $\vec{B} \cdot \hat{n}$ [17], where $\hat{n}$ is normal to the ribbon. The angle between the tangent of each point in MR undergoes a uniform change by assuming a smooth arc in the MR.

To analyze all possible interface and edge states, we choose a graphene ribbon with zigzag edge, where an open (periodic) boundary condition is taken in the $x(y)$ direction, as shown in Fig. 1(a). By diagonalizing the Hamiltonian equation (1) on a rectangular sample under a nonuniform magnetic field, we obtain energy spectrums for different bending angles, shown in the top panel of Fig. 2. Due to the particle-hole symmetry, the electron energy spectrum is symmetrical about zero energy which is similar to that of pristine graphene [1]. However, the band structure of bent graphene is different from the case of pristine graphene in a uniform magnetic field, because the bend changes the distribution of effective

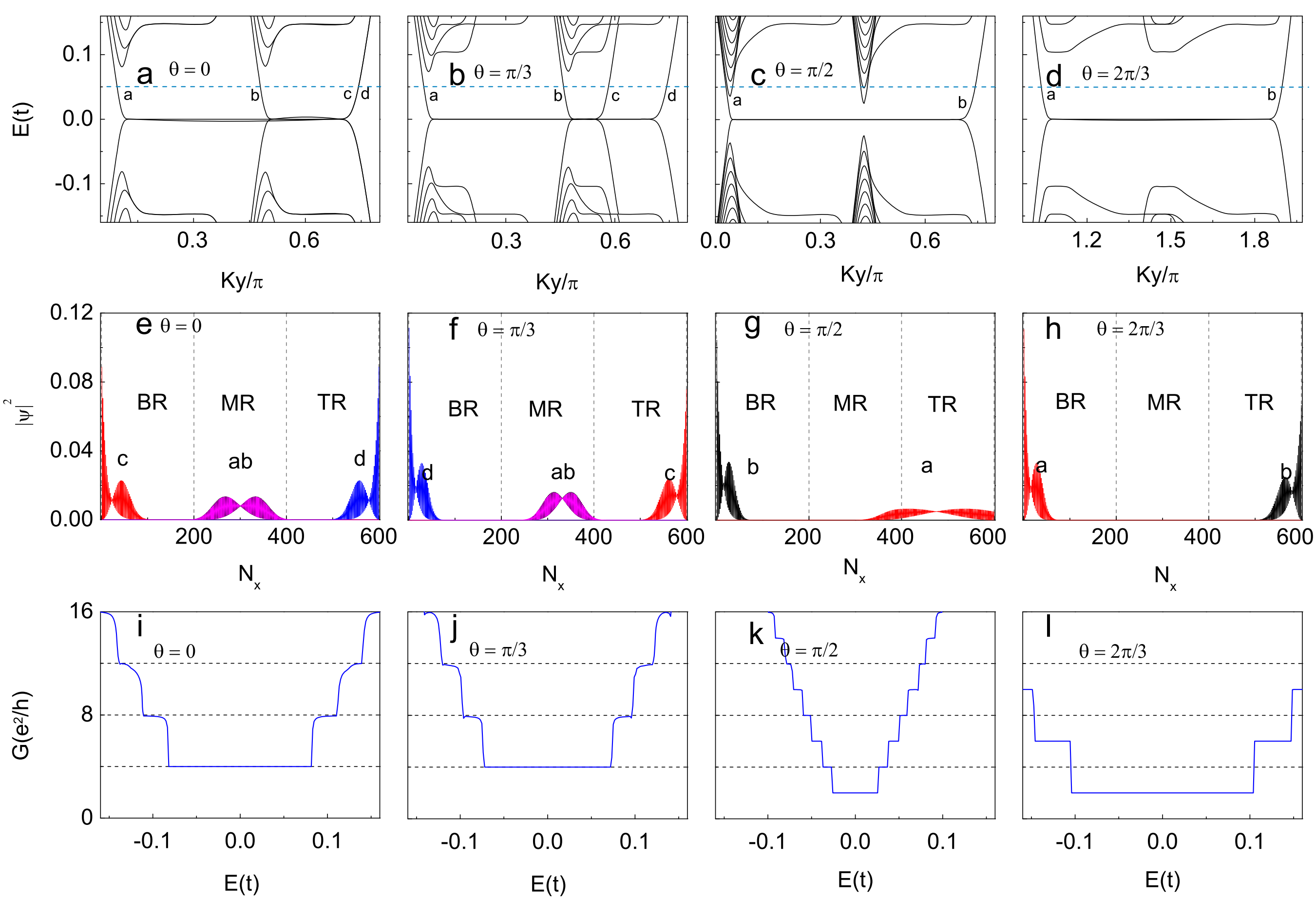

Fig. 2. Top panel: the electron energy spectrum of bent graphene ribbon with $\phi = 0.002$ and $L_x \approx 28.4$ nm. Middle panel: the spatial distributions of interface and edge states indicated in the top panel labelled by the letters a, b, c and d. N_x represents lattice indexes. Bottom panel: the corresponding calculated conductance for the bent graphene ribbon.