Physics Letters A 380 (2016) 3738–3742

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

The opposite induced magnetic moment in narrow zigzag graphene nanoribbons

Hong Liu *, Bian Hu, Na Liu

Physics Department of Nanjing Normal University, Nanjing 210023, China

ARTICLE INFO

Article history:
Received 26 May 2016
Received in revised form 4 September 2016
Accepted 8 September 2016
Available online 12 September 2016
Communicated by R. Wu

ABSTRACT

Based on the analysis of band structure and edge states on zigzag graphene nanoribbons (ZGNRs), we can study theoretically the origination of two minimal quantum conductance. At the two energy points −0.20 eV and 0.15 eV corresponding to the two dips of quantum conductance, the spin-polarized quantum conductance is about 45%. Furthermore, the two types of edge-localized carriers in the opposite transport directions along the two opposite edge sides form the quantum internal loop current, which can generate one big magnetic moment. At these two energy points −0.17 eV and 0.15 eV the two induced magnetic moments are in opposite signals.

1. Introduction

Since the groundbreaking experiments on the monolayer graphene [1], the low-dimensional carbon nano-materials is a promising material for future electronics. The extensive experimental and theoretical researches have been devoted to study their various novel physical properties. The subsequent experimental measurement on graphene layers motivated the investigation on the spin quantum transport in graphene [2,3], especially the quantum anomalous Hall effect (QAHE) [4,5]. Without the spin-splitting factors early many theoretical work investigated the band structure and quantum current, and proposed the massless Dirac dispersion in band structure of various graphene nanoribbons [6–13], the band gap and the zero-energy edge states in the two-dimensional narrow graphene nanoribbons (GNRs) [14–19]. The electronic transport in graphene nanoribbons with sublattice-asymmetric doping [20] and in the heterosubstrate-induced graphene superlattices [21] are investigated recently. Involving the spin-splitting factor, Y.-W. Son et al. found that the band gap and the spin-polarized edge states from the first principle method [22]. J Guo et al. introduced the self-consistent on-site Coulomb interaction (O-CIs) [23,24] into the tight-binding model to successfully obtain the band structure in agreement with the results of Son's work [22]. Furthermore, at the Fermi energy the electrons with different spin spatially distribute on the different edges, respectively, so called spin-polarized edge states in ZGNR [14–28]. These unique features would lead to interesting electronic transport properties. L. Sheng et al. proposed the spin Chern number to determine the various phases of quantum Hall effect [26–28]. The low-bias low-temperature integer-step quantized conductance in graphene nanoribbon with various edges have been studied in the many works of Refs. [7–19,23–27]. Recently, J. Wilhelm et al. studied the spin-flip conductance of hydrogenated graphene nanoribbon from the first principle method [29]. Our previous work successfully studied the binding energy of exciton exciting between two edge states [30] and the quantum current [31] involving this self-consistent O-CIs.

Since the work of Kane and Mele [32,33] in graphene nanoribbon, the spin–orbit couplings (SOCs) have attracted much attention on the edge band and edge states in GNRs. Based on the Kane and Mele (KM) model the integer-step quantized conductance is studied in many theoretical work [26–29,34–38]. Sheng's group proposed a Laughlin-like gauge argument to understand the general properties of edge states [26,27] and reviewed the characteristics of quantum spin Hall effect (QSHE) [28]. By using the KM model, varying the strengths of SOCs, M. Ezawa investigated the quantum phase transition and the quantized conductances in silicene nanoribbons [34,35]. Especially, under low-bias and low temperature J. Baringhaus et al. [40,41] precisely measure the quantum conductance in GNRs with different length and width. At zero-bias the integer of quantized conductance changes from 2 to 0 with the increase of length [40]. The probed transmissions of Farby–Perot-like resonances showed one transport gap 5 meV [41] at low temperature in graphene nanoconstrictions (GNCs) with length

* Corresponding author.
E-mail address: liuhong3@njnu.edu.cn (H. Liu).

http://dx.doi.org/10.1016/j.physleta.2016.09.012
0375-9601/

$L = 6$ nm and width $W = 2$ nm. However, because the strengths of SOCs are very weak in graphene [42,43], the measurement of novel spin-polarized transport can not be achieved in ZGNRs. Therefore, one proposed and developed some methods to open band gap [13, 28,35,39] and to enhance the strengths of SOCs [44–48].

Concerning on the O-CIs, the QHE system can be changed as the change of topological edge bands by adjusting the strength of the O-CIs in ZGNRs [13,28,35,39]. When adding one constant O-CIs term, Wang et al. [39] obtained one different edge band structure from Sheng's work (in Ref. [28]). The unique spin-related electronic structures and the topologically-protected edge states are sensitive to the Coulomb interactions (CIs), especially the O-CIs. Many theoretical works studied the influences of the O-CIs on quantum transport and band structure, such as the CI on the doping site [13], the staggered lattice CI [28,35], and the constant O-CIs [39], however, these types of CIs do not consider the spin-splitting factor and can not compare with the band structure from the first principle method [22]. Obviously, the self-consistent O-CIs [23,24] can provide reasonable band structure having a band gap. As far as we know, one did not use this type of O-CIs together with two types of SOCs and the Zeeman effect to study the band structure of edge states and the spin quantum transport.

In the present work, based on the tight binding KM model [32,33], we think that the self-consistent O-CIs [23,24] can help us understand and predict novel phenomena associated with spin transport due to the existence of the edge states compared with the previous theoretical work [28,39]. According to the edge band structure and the strong localization of electron at the two edges, we think that the two opposite quantum currents at the edges can form of the internal current loop, which can generate strong magnetic moment. Thus it can provide one experimental way to observe the SOCs and the localization characteristics of carriers in the edge states. This paper is organized as follows: In Sec. 2 we outline our theoretical approach. Numerical results are presented and discussed in Sec. 3. We close by providing a brief summary and outlook in Sec. 4.

2. Theoretical approach

Despite the hoping kinetic terms, in the present work, the Hamiltonian of system still involves the two types of spin–orbit couplings (SOCs) describing by the Kane–Mele model [32,33], the Zeeman effect generated by the applied magnetic field and the self-consistent on-site Coulomb potential [20,21]. The Zeeman effect plays an important role to form the edge bands crossing the Fermi energy, in which the electrons of two edge states at the same energy are in the ferromagnetic spin-polarized configuration at the two edges, respectively [49]. The Hamiltonian is written as [23–25,32,33,49,50]

$$\hat{H} = \hat{H}_0 + \hat{H}_{SO} + \hat{H}_Z + \hat{H}_U, \tag{1}$$

where

$$\hat{H}_0 = \sum_{\langle i,j\rangle} t_{ij} c_i^+ c_j,$$

$$\hat{H}_{SO} = iV_R \sum_{\langle i,j\rangle} c_i^+ \mathbf{e}_z \cdot (\boldsymbol{\sigma} \times \mathbf{d}_{ij}) c_j + iV_{so} \frac{2}{\sqrt{3}} \sum_{\langle\langle i,j\rangle\rangle} c_i^+ \boldsymbol{\sigma} \cdot (\mathbf{d}_{kj} \times \mathbf{d}_{ik}) c_j,$$

$$\hat{H}_Z = g \sum_i c_i^+ \sigma_z c_i,$$

$$\hat{H}_U = \sum_{i,\sigma} U \left(\langle n_{i\bar{\sigma}} \rangle - \frac{1}{2} \right) n_{i\sigma},$$

where $c_i^+ = (c_{i\uparrow}^+, c_{i\downarrow}^+)$ ($c_i = (c_{i\uparrow}, c_{i\downarrow})^T$) is the electron creation (annihilation) operator at site i, $\boldsymbol{\sigma}$ is a vector that consists of the Pauli spin matrices. $\sum_{\langle i,j\rangle}$ denotes the summation over the nearest-neighbor sites, the sum $\sum_{\langle\langle i,j\rangle\rangle}$ is restricted to next nearest-neighbor sites, and $t_{ij} = -2.60$ eV is the two-center hopping integral between the nearest neighbor sites. $\mathbf{d}_{ik}$ is a unit vector pointing from site k to site i, where k is the only common nearest neighbor of i and j. The first term is general kinetic term H_0. The second term H_{so} represents the SOCs within the Kane–Mele spin–orbit model [32,33,50]. Whereas involves the Rashba SOC and the intrinsic SOC denoted as H_{so}. The third term H_Z is the Zeeman effect generated by the applied external magnetic field perpendicular to the plane of ZGNR. The Zeeman effect not only can open a band gap, but also can lift the spin-degeneracy [28,35]. The fourth term H_U is the O-CIs [20,21], in which $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$ is the spin-resolved number operator, and $\langle n_{i\sigma} \rangle$ is the average occupation probability of electrons on site i with the spin-direction σ. In the calculation of the Fermi–Dirac distribution we take the room temperature $T = 300$ K. Although the intrinsic SOC is very weak in graphene [42,43], there are some developed methods to enhance it by magnetic adatoms [44,45], impurities [46], substrate [47], and halogeneration [48]. Therefore, in the our calculation we can take the large SOC interaction parameters $V_R = 0.01t_{ij}$, $V_{so} = 0.02t_{ij}$, $g = 0.02$ eV [28] and $U = 4$ eV [20,21] in order to clearly illustrate the spin quantum conductance contributing from the edge states. The width of ZGNR can be defined by the number of sites in the unit cell. In the present work taken the width $N_W = 8$ as an example we investigate the electron structure and the quantum transport.

The conductance through a region of interacting electrons can be calculated by use of the Landauer formula [51–55]

$$\mathcal{T} = \left(\frac{e^2}{h} \right) tr\left(\Gamma_L G_C^r \Gamma_R G_C^a \right), \tag{2}$$

where $tr(\Gamma_L G_C^r \Gamma_R G_C^a)$ is the transmission function, $G_C^{r,a}$ represent the retarded and advanced Green function of the heterojunction, and $\Gamma_{L,R}$ are the couplings of the heterojunction to the left and the right ZGNRs, respectively. In the present work the heterojunction and the two leads adopt the same periodic length with one layer of ZGNR to self-consistently calculate the O-CIs on site in Eq. (1). Therefore, the calculated quantum conductance is for an ideal crystal.

The internal current from site j to i is calculated from the Green's function G^n, usually referred to as a correlation function [56–58],

$$I_{ij} = \frac{e}{h} \mathbf{Im}[H_{ij} G_{ij}]. \tag{3}$$

The correlation function G^n is defined as $G^n = G_C^r \Gamma_L G_C^a$. The magnetic moment arising as a result of the quantum loop current also has interesting properties. Recall that the induced magnetic moment is expressed as,

$$\mathbf{M} = \sum_{\langle i,j\rangle} I_{ij} (\mathbf{r}_i \times \mathbf{r}_j)/2, \tag{4}$$

where the summation is taken over each pair, i and j, whose corresponding Hamiltonian matrix element is nonzero, and $\mathbf{r}_i$ indicates the coordinates of the site i. Due to $\mathbf{r}_i$ in the plane of ZGNR the magnetic moment has only the z-component.

3. Results & discussion

3.1. Band structure and edge states

Firstly, we show the band structure and the electron spin spatial distributions of edge bands near the Fermi energy in order