Straintronics in graphene nanoribbons: the appearance of the middle “edge states”

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Strain can tailor the band structures and properties of graphene nanoribbons (GNRs) with the well-known emergent pseudo-magnetic field and the corresponding pseudo-Landau levels (pLLs). We design one type of strained zigzag GNR (ZGNR) which supports the “edge states” propagating in the middle of the sample. The fascinating point is that the pseudo-magnetic fields with opposite directions between the lower and upper half planes are induced by the strain. Therefore, the electrons experience the opposite Lorentz forces and change the direction of rotation when they arrive at the border line between the upper and lower half planes, which prompts the propagation of the middle “edge states”. By using the Landauer-Büttiker formalism combined with the nonequilibrium Green’s function method, the existence and robustness of the middle “edge states” are further studied. Furthermore, the realization of long-thought pure valley currents in monolayer graphene systems is also proposed in our device.

I. INTRODUCTION

Graphene, a single-atom-layer carbon material, has the peculiar band structure with two nonequivalent Dirac points $K$ and $K'$, leading to a pseudo-spin degree of freedom, i.e., valley [1–3]. The field utilizing the valley degree of freedom is referred to as valleytronics [4], which takes advantage of graphene and gapped 2D Dirac materials [5–7]. Graphene nanoribbons (GNRs), cut from the graphene, are quasi-one-dimensional systems. There are two basic shapes for GNR edges — zigzag and armchair edges, and more specially, the zigzag GNRs (ZGNRs) support zero-energy flat bands of edge states [8–11]. In our work, we mainly focus on the ZGNRs. Straintronics, a new discipline developed in recent decades, utilize strain engineering methods and strain-induced physical effects to develop novel functional devices [12–14]. Because the graphene has the outstanding capability to sustain nondestructive reversible deformations up to high values 25% to 27% [15–18], it can be a good candidate for making novel strain devices [19]. One of the most remarkable properties induced by the strain in graphene is the appearance of the pseudo-magnetic field and the corresponding pseudo-Landau level (pLLs) [20–28], which have been observed in several excellent experiments [29–34].

Previous work usually consider the model shown in Fig. 1(a) [24, 31, 35], where the ZGNR is stretched along the $y$ direction, and assuming the hopping coefficients are constant along the $x$ direction but decreasing successively from the lower edge to the upper one. Obviously, stretching increase the bond lengths, thus it will decrease the hopping coefficients which depend on the overlap integral of wave functions belonging to neighbouring sites. As a result, we call this strain pattern the monotone increasing strain (MIS), and if the hopping coefficients decreases
linearly, a uniform perpendicular pseudo-magnetic field emerges and acts on the electrons locally, leading to the specific dispersive pLLs [24, 35]. Even though the ZGNRs with MIS are charming and well-studied, we suppose that another strain pattern shown in Fig. 1(d) may be more easier to realize. It is clearly that the ZGNR with symmetrical structures in Fig. 1(d) can be viewed as two copies of the ZGNR in Fig. 1(a) where the lower copy \((y < 0)\) is the horizontal inversion partner of the upper copy \((y > 0)\). The corresponding strain pattern we named the symmetrical strain (SS). It should be pointed out that even though we call it SS and the structure in Fig. 1(d) respects the inversion symmetry, the accurate symmetry between the lower and upper planes is not necessary. To be precise, what we need is the uniaxial strain with opposite directions between the lower and half planes.

Because of the Newton’s third law of motion, i.e., all forces between two objects exist in equal magnitude and opposite direction, we can expect that the ZGNR with SS may be more natural to fabricate than the ZGNR with MIS. For instance, if the ZGNR is stretched along the \(y\) direction, and the \(n_y = 1\) and \(n_y = N_y\) edges are fixed by probes or substrates, the SS pattern maybe form naturally. Polarized valley currents are predicted in the ZGNR with MIS [35], so the meaningful question is what form should the valley currents present in the ZGNR with SS. Interestingly we found that except for the ordinary edge states propagate in the actual edges, the similar “edge states” can flow in the middle of the sample, which constitutes a new type of quantum valley Hall effect (QVHE) where exists the middle “edge states”. Even though the middle “edge states” may be viewed as the bound states near the domain wall — 1D “line defect” along the \(y = 0\) line — between the lower and upper half parts, they are still fascinating because: (i) this 1D “line defect” is natural and “invisible”, and we don’t need to dope any real impurities; (ii) the middle “edge states” come from a fascinating phenomenon — the pseudo-magnetic fields have opposite directions between the lower and upper half parts, which is the result of the SS.

The paper is organized as follows. Sec. II, we show the formation mechanism of the middle “edge states”. In Sec. III, we propose that the pure valley currents exist in the ZGNR with SS, which can be measured through the charge transport. In Sec. IV, we verify the existence of the middle “edge states” by the conductance of the two-terminal device calculated by the Landauer-Büttiker formalism and nonequilibrium Green’s function method, and discuss the robustness of the middle “edge states”. Sec. V is the conclusion.

II. THE NOVEL MIDDLE “EDGE STATES”

The Hamiltonian in the tight-binding representation of the strained ZGNRs is \(H = \sum_{i} \varepsilon_i a_i^\dagger a_i - \sum_{<ij>} t a_i^\dagger a_j\), where \(\varepsilon_i\) is the onsite energy, \(a_i^\dagger\) and \(a_i\) represent the creation and annihilation operators. For simplicity, we only consider the nearest-neighbor hopping, neglecting the next-nearest-neighbor hopping [35]. The strain strength is included in the hopping coefficient \(t\), e.g., \(t_y = t_0 (t_y = t_0 (1 - \eta))\) is corresponding to the hopping coefficient between the \(n_y = 1\) and \(n_y = 2\) \((n_y = N_y - 1\) and \(n_y = N_y\)) chains in Fig. 1(a). Here \(t_0 = 2.75\) eV is well-known hopping coefficient for the normal graphene [36], and \(\eta\) is an adjustable variable which reflects the strain strength. In the following calculations, we take \(\eta = 0.5\), which can be achieved in the experiments. First, we know that the graphene can sustain nondestructive reversible deformations up to high values 25% to 27% [15–18]. Second, previous work has presented this relation \(t_y = t_0 \exp[-\beta (t/a_0 - 1)]\) [18], where \(\beta = 1.25 a_0\) for the deformation value 25%, we will get \(t_y = 0.43 t_0\), which suggests that the strain strength \(\eta = 0.5\) falls in the nondestructive reversible region.

Fig. 1(b) shows the band structure of the ZGNR with MIS in Fig. 1(a) with \(N_y = 80\) and \(\eta = 0.5\). In our calculations, the hopping coefficients are supposed to be constant and decreasing linearly along the \(x\) and \(y\) direction, respectively [25]. As a result, the difference of \(t_y\) between neighboring carbon atoms along the \(y\) direction is approximately 0.6%. It is clearly that the dispersive pseudo-Landau levels form in the low energy regime, which is consistent with Ref. [25, 35]. In order to explore the probability distributions of the wave functions belonging to each band, we analyze the situations for selected \(k\) points. Typical results are demonstrated in Fig 1(c), where we have chosen the \(k\) points A-F at the intersections of the energy line \(E = 0.33\) eV and the lowest energy bands in Fig. 1(b). It is clearly shown that the wave functions associated with points A and C distribute near the lower and upper edges, respectively. As a comparison, the wave function of point B spreads into the bulk. We have checked that the wave functions of adjacent \(k\) points near A, B, C have the similar localized properties with them. Additionally, the band structures and wave functions associated with D, E, F are the same with that of C, B and A, which is shown in Figs. 1(b) and (c).

Fig. 1(e) shows the band structure of the ZGNR with SS in Fig. 1(d) with \(N_y = 160\) and \(\eta = 0.5\). The most different between the ZGNR with SS and the one with MIS is the former possesses opposite uniaxial strain between the lower and half planes, which provides the possibility for the middle “edge states” discussed below. Similar to Fig. 1(b), the \(k\) points A-H at the intersections of the energy line \(E = 0.33\) eV and the lowest energy bands are chosen in Fig. 1(e). Combined with the results in Fig. 1(f), we can see that the wave functions associated with points A and H (D and E) moves to the middle position (new edges). This result can be easily understood
since the wave functions associated with point A (C) distribute near the lower (upper) edge which holds no strain strength (the max strain strength). In the ZGNR with SS in Fig. 1(d), the distributions follow the same rule, i.e., the wave functions associated with points A and H (D and E) distribute around the positions with no strain strength (the max strain strength). Similarly, the wave function associated with points B, G, C and F spreads into the bulk. In addition, from the partial enlarged diagram in Fig. 1(e) we can see that, the first pLL splits into band 2 and band 3 at point N due to the boundary condition [37]. Accordingly, a minimal point M emerge, and the surround band in the orange dotted rectangle will contribute additional edge states when the Fermi level across.

FIG. 2. (a) and (b) show the QH edge states; (c) and (d) show the QVH edge states which contain the middle “edge states”.

It should be pointed out that the two valleys \( K \) and \( K' \) are decoupled in the low-energy limit making the study on the valley transport meaningful, as long as no scattering terms can connect the two valleys. As a result, if the Fermi energy lies between adjacent pLLs, the edge states with valley degree of freedom will dominate the transport. We compare the differences between edge states in our model and that in the normal quantum Hall (QH) states in Fig. 2. Fig. 2(a) shows the schematic diagram of the normal QH edge states for one spin species. Electron take circular motions under the perpendicular magnetic fields due to the Lorentz forces. However, electrons near the edges don’t have enough space to complete a circle and will be reflected by the boundary to start another circle, which leads to the 1D chiral edge states. Fig. 2(b) shows the schematic diagram for both spin species.

Next we focus on our device and clarify the mechanism for the formation of the middle “edge states”. The key point is that the directions of the pseudo-magnetic fields are opposite between the upper and lower half planes. As we can see, the directions of the uniaxial strain between the lower (\( y < 0 \)) and upper (\( y > 0 \)) half planes are opposite. Previous work has demonstrated the direction of pseudo-magnetic field is determined by the direction of strain [23], thus it changes immediately at \( y = 0 \). Therefore, the electrons experience the opposite Lorentz forces and change the direction of rotation by turns when they arrive at the border line \( y = 0 \). This is the origin of the middle “edge states”. The above process is clearly shown in Fig. 2(c) for one valley species. The picture for both \( K \) and \( K' \) valleys are illustrated in Fig. 2(d).

Here we emphasize three specific aspects of our model. (i) The pseudo-magnetic field possesses particular different characteristics from the real magnetic field. First, the pseudo-magnetic field respects the time-reversal symmetry and has opposite signs for \( K \) and \( K' \) valley [25]. Second, the effect of the pseudo-magnetic field is local. We know that the real magnetic field can be depicted by magnetic line of force, which means the magnetic force are relevant between different points in space. Thus it is difficult to apply different magnetic fields on different parts of the sample independently. However, the pseudo-magnetic field is an emergent effect depending on the local strain, as a result, it generated by the strain in the vicinity of one point is irrelevant to that generated at other spatial points. Therefore, the pseudo-magnetic fields with opposite directions on the lower and upper half planes evolve naturally and independently. (ii) Why do we call they “edge states” even though they are propagating in the middle of the sample? From Fig. 2(c) and (d) we can see that the currents propagate along the actual edge and middle “edge” in circles. From this point of view, the middle “edge” has no difference from the actual edge. (iii) This is a new type of QVHE. Under the action of the time-reversal-invariant pseudo-magnetic field, the currents of different valleys propagate in opposite directions, and the whole system can be viewed as two copies of conventional QVH states.

III. PURE VALLEY CURRENTS

FIG. 3. Schematic diagram showing (a) two-terminal and (b) four-terminal measurement geometries. In (a) a charge current \( I^c = 4e^2V/h \) flows into the right lead. In(b) a valley current \( I^v = e^2V/h \) flows into the right lead.

The generation of pure valley currents has attracted lots of attention in the past few years. Several theoreti-
cal schemes, e.g., optical excitations \[38\], quantum pumping \[39, 40\], cyclic strain deformations \[41\], and applying AC bias \[42\], have been proposed for realizing pure valley currents. In the laboratory, pure valley currents also have been observed in graphene superlattice \[43\] and graphene bilayers \[44–46\]. However, pure valley currents are very difficult to be observed in the monolayer graphene \[35\].

Using similar methods in Ref. \[47\] in which pure spin currents are discussed, we use the Landauer-Büttiker formula to discuss the valley currents in two and four terminal devices shown in Fig. 3. Different from the usual quantum Hall and quantum spin Hall effect where the 1D conducting states localizing in the edges, the middle “edge states” exist in our device and contribute to transport. According to the Büttiker formula \[48\], the current in \(i\)-th terminal in the equilibrium is

\[
I_i^v = e^2 \hbar \sum_{j \neq i} \left( T_{ji}^c V_i - T_{ij}^c V_j \right),
\]

where \(V_i\) is the voltage in the \(i\)-th terminal and \(T_{ji}^c\) is the transmission coefficient for valley \(\sigma (\sigma = K, K')\) between the \(i\)-th and \(j\)-th terminals. Naturally, the charge current and valley current can be defined by \(I_i^c = I_i^K + I_i^{K'}\) and \(I_i^v = I_i^K - I_i^{K'}\).

For the two-terminal device shown in Fig. 3(a), \(T_{34}^c = T_{43}^c = 2\), thus we get \(I_2^c = (2V_1 - 2V_2) e^2 / h\) and \(I_2^v = (2V_1 - 2V_2) e^2 / h\) for terminal 2. If we take \(V_1 = V/2\) and \(V_2 = -V/2\), then \(I_2^c = 2e^2 V/h\) and \(I_2^v = 2e^2 V/h\). As a result, \(I_2^c = 4e^2 V/h\), \(I_2^v = 0\). This suggests that the pure valley currents cannot exist in the two-terminal device. Next we study the four-terminal device shown in Fig. 3(b) to see whether the pure valley currents can survive. In this case, the transmission coefficients for \(K\) valley currents are \(T_{34}^c = T_{43}^c = T_{24}^c = T_{42}^c = 1\), \(T_{34}^v = T_{43}^v = 2\) and 0 otherwise; the transmission coefficients for \(K'\) valley currents are \(T_{34}^c = T_{43}^c = T_{24}^v = T_{42}^v = 1\), \(T_{34}^v = T_{43}^v = 2\) and 0 otherwise. Therefore, we can get \(I_2^c = (V_1 + V_2 + V_3 - 4V_4) e^2 / h\) and \(I_2^v = (V_1 + V_2 - V_3) e^2 / h\). If we take \(V_1 = -V/2\), \(V_2 = V/4\), \(V_3 = V_4 = 0\), we have \(I_2^c = 0\) but \(I_2^v = 2e^2 V/h\), which suggest that we can obtain the pure valley currents in terminal 4. In other words, the pure valley currents can be measured through the charge transport in a mesoscopic system as shown in Fig. 3. It should be pointed out that this is one simple and elegant way to realize the pure valley currents in the monolayer graphene systems.

IV. CONDUCTANCES FROM THE “EDGE STATES”

Next we use the nonequilibrium Green’s function method to calculate the conductance of the strained ZGNR shown in Fig. 4(a), which can clearly illustrate the middle “edge states” exist or not. The linear conductance of the strained ZGNR is \(G = \lim_{V \to 0} dI/dV\), where the current \(I\) is obtained by the Landauer-Büttiker formula \(36, 49\): \(I = (2e/h) \int d\varepsilon \mathcal{T}_{LR} (\varepsilon) \{ f_L (\varepsilon) - f_R (\varepsilon) \}\). Here \(f_L = 1/\{ \exp [ (\varepsilon - eV) / k_B T] + 1 \}\) is the Fermi function of the \(\alpha (\alpha = L, R)\) lead, and \(\mathcal{T}_{LR} (\varepsilon) = \text{Tr} (\Gamma_L G^R \Gamma_R G^\alpha)\) is the transmission coefficient with the linewidth functions \(\Gamma = i \{ \Sigma_{\alpha} (\varepsilon) - \Sigma_{\alpha}^* (\varepsilon) \}\) and the self-energy \(\Sigma_{\alpha}^{\text{self}}\). The retarded and advanced Green’s function is \(G^R (\varepsilon) = 1/ [\varepsilon - H_{\text{cen}} - \Sigma_{\alpha} (\varepsilon)]\) and \(G^\alpha (\varepsilon) = [G^R (\varepsilon)]^\dagger\), respectively, where \(H_{\text{cen}}\) is the Hamiltonian of the central region. In the following numerical calculations, we take the hopping energy \(t_0 \approx 2.75\) eV, and since the \(t_0\) corresponds to \(10^4\) K, we can safely set the temperature to zero in our calculations \(36\). Fig. 4(a) shows the schematic diagram of the device we studied. The left and right lead are semi-infinite long, and the central part has the width \(N_y = 160\) and length \(N_x = 60\), which means that there are 60 primitive cells in the \(x\) direction.

We first study the clean strained ZGNRs. Fig. 4(b) compare three strain patterns: the blue dash-dot line shows the conductance without strain, which is quantized and exhibits a series of equidistant plateaus due to the transverse sub-bands of the ZGNR with finite width. The green dot line corresponds to the conductance of the
ZGNR with MIS. It is clearly that due to the formation of the pLLs, the width of the lower plateaus increase. Furthermore, the step interval of the plateaus maintains $4\epsilon^2/h$ which is attributed to the states located in the two edges. After we introduce the SS, the step interval of the plateaus increases to $8\epsilon^2/h$, which implies the formation of the middle “edge states”. It should be pointed out that two peaks $P_1$ and $P_2$ emerge on the second and third plateaus due to the energy bands inside the orange dot rectangle in Fig.1(e). In fact, $P_1$ and $P_2$ are two narrow plateaus which is clearly shown in Fig.4(f). From Fig.1(c) we can see that the points similar with the emergent minimum point N are more difficult to appear on higher pLLs, thus the strengths of the similar narrow plateaus become smaller with increasing $E_F$.

In fact, the strain strength plays the role of the pseudo-magnetic field, contributing to the pLLs and the quantized valley Hall conductance. Therefore, we plot Fig.4(c) to illustrate the conductance with the change in strain, which shows the evolution of step interval from $4\epsilon^2/h$ to $8\epsilon^2/h$. Blue dot line corresponds to the ZGNR without strain, and according to the above analysis, the step interval is $4\epsilon^2/h$. The green dot line, purple dot line and the red solid line present the conductances versus the increase of strain. It is clearly shown that along with the increase of strain, the plateaus at $6\epsilon^2/h$, $14\epsilon^2/h$, $22\epsilon^2/h$, $30\epsilon^2/h$ become narrower. Until they disappear, the step interval between adjacent plateaus changes from $4\epsilon^2/h$ to $8\epsilon^2/h$. Meanwhile, $P_1$ and $P_2$ appear gradually because of the formations of new edge states.

Next we examine the effect of disorder on the middle “edge states”. In the following calculations, we suppose that the disorder only exists in the central region, and in the presence of disorder, we take 500 random configurations and calculate the average values of the conductances. Since this procedure has high computation cost, we cannot take the same number of $E_F$ as that in Fig.4(b) and (c). However, to avoid missing information related to $P_1$ and $P_2$, we take more number of $E_F$ around them in the calculations. The detailed results are illustrated in Fig.4(d) and the drawing of partial enlargement of the first plateau, $P_1$ and $P_2$ are shown in Fig.4(e) and (f), respectively. The results can be summarized as follows: (i) when the strength of disorder is very weak, e.g., $w \leq 0.1$ eV, all plateaus, except for $P_1$ and $P_2$, maintain well. $P_1$ and $P_2$ are not robust because the range of band structure inside the orange dot rectangle in Fig.1(e) is small. Moreover, this type of peaks will become more fragile on higher plateaus. (ii) When the strength of disorder increase, e.g., $w = 0.5$ eV, only the first plateau is robust. It is noted that there is a minimum of conductance in the vicinity of $E_F = 0$ in Fig.4(d) and (e). This is due to the large density of states of the flat $n = 0$ pLL and the nonequilibrium Green’s function method can not accurately calculate the conductance in this small region. The physical reason why the conductance plateaus is not so robustness is the middle “edge states” are easy to become hybrid due to the close distance between them in the real space. Therefore, we need to explore schemes preventing the hybridization and obtain more robust middle “edge states”.

V. CONCLUSIONS

The valley degree of freedom attributed to the non-equivalent Dirac points $K$ and $K'$ is well-known for decades. Furthermore, strain can be used to tailor the band structures and properties of the ZGNRs, and the most charming phenomenon is the emergent pseudo-magnetic field and the corresponding pLLs. In order to explore new types of pure valley currents, we design the strained ZGNR which can support the “edge states” propagating in the middle of the sample. We point out that the uniaxial strain with different directions between the lower and half planes is the essential ingredient for the formation of the middle “edge states”. Based on our design, we can use a four-terminal device to realize the long-thought pure valley currents in monolayer graphene systems. Furthermore, we calculate the conductance of the two-terminal device, obtaining the $8\epsilon^2/h$ step interval between neighbouring plateaus, which indicates the formation of the middle “edge states”. By introducing the Anderson impurities, we find that the first conductance plateau is more robust than higher plateaus. One obstacle to the robustness of the middle “edge states” is they are easy to become hybrid due to the close distance between them in the real space. One of the next aim is to explore schemes preventing the hybridization and obtain more robust middle “edge states”.

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